DOE/SC-0061

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2001

August 8, 2002

Annual Technical Report

U.S. Department of Energy
Office of Science
Office of Basic Energy Sciences
Division of Materials Sciences
Germantown, MD 20874-1290

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INTRODUCTION

The DOE Energy Materials Coordinating Committee (EMaCC) serves primarily to enhance coordination among the Department's materials programs and to further effective use of materials expertise within the Department. These functions are accomplished through the exchange of budgetary and planning information among program managers and through technical meetings/workshops on selected topics involving both DOE and major contractors. In addition, EMaCC assists in obtaining materials-related inputs for both intra- and interagency compilations.

Six topical subcommittees have been established to focus on materials areas of particular importance to the Department; the subcommittees and their respective chairpersons are:

Electrochemical Technologies - Richard Kelly, SC-13 (301) 903-6051
Metals - Sara Dillich, EE-22 (202) 586-7925
Radioactive Waste Containers - Matesh (Mat) Varma, SC-13 (301) 903-3209
Semiconductors - Jerry Smith, SC-13 (301) 903-4269
Structural Ceramics - Charles Sorrell, EE-23 (202) 586-1514
Superconductivity - James Daley, EE-15 (202) 586-1165

Membership in the EMaCC is open to any Department organizational unit; participants are appointed by Division or Office Directors. The current active membership is listed on pages 3-5.

Five meetings were scheduled for 2001-2002. The dates and minutes from the meetings are as follows:

SEPTEMBER 26, 2001, 10:15 A.M.-12:20 P.M., ROOM G-207/GTN

This meeting was originally scheduled for September 11, 2001, at the Forrestal building. The chairman, Dr. Matesh Varma, opened the meeting by first observing a moment of silence for the victims of the events on September 11. He then continued by having the participants introduce themselves and state their affiliation.

Dr. Sam Berk from the Office of Fusion Energy Sciences (OFES) described the materials sciences efforts for fusion energy. Their Fusion Materials Research has a budget of $8.6M for FY2001. Their major materials problems concern the first wall and blanket that surround the plasma chamber. These must withstand a high temperature heat load and a heavy flux of 14MeV neutrons without spalling heavy contaminants into the plasma. Additional information is available on the Internet:

Fusion Energy System Concepts: http://aries.ucsd.edu/ARIES
Fusion Materials Research: http://www.fusionmaterials.pnl.gov
Chamber Technologies: http://www.fusion.ucla.edu/APEX
Plasma Facing Components : http://www.td.anl.gov/ALPS_Info_Center

The last three entries represent projects now subject to peer review. The results of the most recent reviews are available at: http://vlt.ucsd.edu/peer.html.

Prof. Bruce N. Harmon was to present a talk on the Computational Materials Sciences Network (CMSN) which he coordinates. Although he was present for the aborted September 11 meeting, he had schedule conflicts with the rescheduled meeting. So Dr. Dale Koelling substituted. Conceptually, CMSN is a center without walls that assembles Cooperative Research Teams of widely dispersed researchers to tackle larger, more complex problems. The research is funded by the researchers' base program. CMSN provides the "glue" funds to cover the extra costs of collaboration. Further information is available on the Internet at http://cmpweb.Ameslab.gov/CMSN.

Joe Carpenter informed us of the 16th annual National Educators Workshop to be held October 14-17, 2001, at the National Institute of Standards and Technology. The purpose of the workshop is to provide modern examples of materials sciences to educators at the undergraduate level. He also pointed out that this is the last year of NIST's 3-year sponsorship and that a new sponsor is being sought.

The final item of business was to confirm and install the new chairman, Dr. Udaya Rao, and secretary, Dr. Dale Koelling.

CALENDAR ITEMS

(A number of events were announced at the meeting and more have been added. We will include all relevant events that members convey to us.)

October 8-10, 2001:	BES review at Lawrence Berkeley National Laboratory, contact Dr. W. Oosterhuis
November 12-14, 2001:	BES review at Argonne National Laboratory, contact Dr. Helen Kerch
November 13-14, 2001:	BES review at Los Alamos National Laboratory, contact Dr. Yok Chen
November 14-15, 2001:	Basic Energy Sciences Advisory Committee, contact Sharon Long
December 5-7, 2001:	BES review at Brookhaven National Laboratory, contact Dr. Helen Kerch
December 17-18, 2001:	Council on Materials Sciences, Gaithersburg, contact Christie Ashton
June 13-14, 2002:	Annual meeting (and review) of the Center for Synthesis and Processing, Gaithersburg, contact Robert Gottschall

LIST OF PARTICIPANTS

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JANUARY 15, 2002,10:15 A.M.-11:45 A.M., ROOM E2-081/FORS

Chairman, Dr. Udaya Rao, opened the meeting by having the participants introduce themselves.

J.J. Smith discussed NSET: Nanoscale Science, Engineering and Technology. The scope applicable to the initiative is described by the brochure *Nanoscale Science, Engineering and Technology Research Directions.* Funds available this year are $8M that will be split between the two divisions of Basic Energy Sciences with parallel calls for national laboratories and for contract research. (In FY2001, $16.1M was placed in contract research and $10.4M plus nanocenter pre-design funding was placed at the laboratories.) Announcements are on the web. Laboratory applications are due January 18, 2002 and contract research applications are due February 12, 2002.

C. Mailhiot briefly discussed the NNSA effort on physics-based multiscale modeling and then introduced V. Bulatov.

V. Bulatov presented an example of such physics-based multiscale modeling by discussing “Crystal Plasticity from Defect Dynamics.” The presentation was organized about the two keywords *computability* and *fidelity*. Computability refers to the fact that the computation of real properties requires a significant stretch of capabilities. A key to a solution is encapsulated in his statement: “Crystals are like people—it is the defects that make them interesting.” Fortunately, defects are far less dense than the atoms. So one can perform atomistic calculations and pass the information (both conceptual possibilities for behavior and quantitative parameters) to defect-based calculations that hide the presence of the atoms. They have been able to achieve simulations with the requisite 10^6-10^7 dislocations using a combination of massively parallel computing and algorithm change. For reference, current state of the art codes typically accommodate about 40,000 defects. A concrete accomplishment has been to show that networks of screw dislocations move conservatively at much lower stress than the individual dislocations. The result is expected to support a significant rethinking of plasticity theory. The other major objective is to be able to run the simulations for a long enough time to build up a 10 percent strain. This degree of deformation is needed to observe the various self-organizations that might occur. Current state of the art is capable of about 0.2 percent strain. This is the issue currently being addressed. Fidelity refers to the requirement that the calculations agree with experiment. Obviously computability without fidelity is of very limited use. The experimental data is very hard to get and are available only in limited cases. However, the agreement is good where comparisons can be made. With that validation, the calculations permit the investigator both to dissect what is actually occurring and to get information for those cases where experiment is not available.

CALENDAR ITEMS

Jan. 17-19, 2002:	Workshop on New Materials Science Enabled by *In-Situ* Microscopies, Half Moon Bay, CA, contact A. Carim
Mar. 18-22, 2002:	BES/NE Joint Workshop on High Temperature Materials for Nuclear Reactors, La Jolla, contact M. Kassner
Mar. 27-28, 2002:	Joint meeting of Solid State Sciences Committee and National Materials Advisory Board, National Academy of Science, contact R. Gottschall or W. T. Oosterhuis
April 22-26, 2002:	Annual Fossil Energy Materials Workshop, Baltimore, contact Udaya Rao (dates will be refined)
May 6-7, 2002:	Metals and Ceramics Sciences Peer Review, Brookhaven National Laboratory, contact T. Fitzsimmons
May 7-9, 2002:	Workshop to Define Scientific Issues in Multiphase Flow, Urbana, IL, contact B. Armaly
May 16-17, 2002:	Metals and Ceramics Sciences Peer Review, Ames Laboratory, contact T. Fitzsimmons
May 21-22, 2002:	Energy Sciences Nanosciences Symposium, Argonne National Laboratory, contact R. Gottschall
May 21-22, 2002:	BES-NNSA Nanosciences Network Review, Argonne National Laboratory, contact R. Gottschall
June 3-5, 2002:	Metals and Ceramics Sciences Peer Review, Oak Ridge National Laboratory, contact T. Fitzsimmons
June 13-14, 2002:	Annual meeting (and review) of the Center for Synthesis and Processing, Gaithersburg, contact R. Gottschall

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APRIL 16, 2002, 10:20 A.M.-11:40 A.M., ROOM E401/GTN

Chairman, Dr. Udaya Rao, opened the meeting by having the participants introduce themselves.

Iran Thomas (BES) discussed planning for a *Workshop on Basic Energy Needs for Energy Technologies* to occur in the October time frame. This workshop is one step in responding to a major shift in our mission. When our precursor ERDA was formed, the main concern was on energy supply. Now, increasing concern about global climate change is a new driver. Roughly 85 percent of our energy is derived from fossil fuels with no significant change in sight. Nuclear energy has been stymied by lack of public acceptance. So improving efficiencies has carried us through the last 20 years. Even greater improvements will be needed! This workshop is being organized to document what is currently available and realistically assess what is feasible. From this, near and long term Basic Energy Science research needs are to be identified. The workshop is to be chaired by John Stringer (EPRI) and Linda Horton (ORNL), vice chair. Participants are to be a mix of scientists, engineers, and representatives from the offices. Suggestions for participants are requested (name, institution, contact and e-mail address).

Glenn H. Bowser (Office of Security) discussed *Technology Development for Counter-Terrorism Application.* He discussed the Safeguards and Security Technology Development Program. They solicit needs from the field and first try to determine if solutions already exist. If not, project proposals are requested from the laboratories. Interagency solutions are sought wherever possible. Generally, what is sought is a device. Materials are unlikely to be the primary objective although they can be a factor. An example where materials have been a major factor is the development of frangible non-lead ammunition.

The minutes of the January 15 meeting were approved and possible dates for the meeting in July were discussed. The meeting was then adjourned.

CALENDAR ITEMS

April 22-24, 2002: Annual Fossil Energy Materials Workshop, Baltimore, contact Udaya Rao
May 6-7, 2002: Metals and Ceramics Sciences Peer Review, Brookhaven National Laboratory, contact T. Fitzsimmons
May 7-9, 2002: Workshop to Define Scientific Issues in Multiphase Flow, Urbana, IL, contact B. Armaly
May 16-17, 2002: Metals and Ceramics Sciences Peer Review, Ames Laboratory, contact T. Fitzsimmons
May 21-22, 2002: Energy Engineering Sciences Nanosciences Symposium, Argonne National Laboratory, contact B. Armaly
May 21-22, 2002: BES-NNSA Nanosciences Network Review, Argonne National Laboratory, contact R. Gottschall
June 3-5, 2002: Metals and Ceramics Sciences Peer Review, Oak Ridge National Laboratory, contact T. Fitzsimmons
June 13-14, 2002: Annual meeting (and review) of the Center for Synthesis and Processing, Gaithersburg, contact R. Gottschall
July 22-23,2002: Basic Energy Sciences Advisory Committee meeting, Gaithersburg, MD, contact Sharon Long
Nov. 5-6,2002: Basic Energy Sciences Advisory Committee meeting, Gaithersburg, MD, contact Sharon Long

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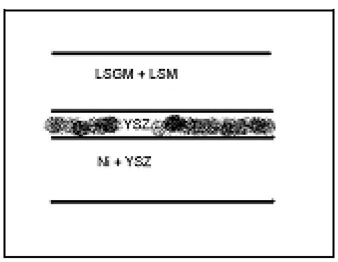
JULY 16, 2002, 10:14 A.M.-11:20 A.M., ROOM GH-019/FORS

Chairman, Dr. Udaya Rao, opened the meeting by having the participants introduce themselves.

Lane Wilson discussed *Materials Issues in the Development of Solid Oxide Fuel Cells*. The Solid State Energy Conversion Alliance (SECA) has the goal of reaching a cost of $800/kW in 2005 and $400/kW in 2010 (which would be commercially competitive). This is to be done with a device having a useful lifetime of 4-8 years. SECA will have a solicitation for broad based fundamental research support.



The basic working element of a solid oxide fuel cell is a trilayer structure as shown in the figure. The top cathode layer must be porous to allow good transport of oxidizing feed gas. The bottom anode layer must transport the fuel gas. They must also provide good electrical and heat transport. The central very thin (Y substituted Zirconia or Sm substituted ceria) layer must allow O^{2-} transport through the layer while blocking H^{+}—the objective is electrochemical charge transfer, not combustion! Both top and bottom layers must provide robust connection to current carrying leads. There are numerous critical materials issues. For example, raising the temperature to get better conductivity oxidizes metal electrical connections and thermally stresses seals and interfaces. One approach for optimizing low temperature operation is a functionally graded electrode utilizing both chemical and microstructure adjustment. Another area of research concerns the anode where oxide and sulfur tolerance is an issue as these ever-present impurities poison the activity of the cell and limit the range of fuels that can be used.

Marshall Reed discussed *Challenges of High Temperature Superconductivity*. Making this presentation was somewhat a heroic effort since they started their annual superconductivity review the next day. The following materials were briefly discussed:

Material	Symmetry	Anisotropy	Transition Temperature (T_c)

$Nb_{53}Ti_{47}$	cubic	---	9
Nb_3Sn	cubic	---	18
MgB_2	hexagonal	2-2.7	39
$YBa_2Cu_3O_{7-x}$	orthorhombic	7	92
$Bi_2Sr_2Ca_2Cu_3O_{9-x}$	tetragonal	50 to 100	108

But the main focus was on the high-T_c materials where meter-long wires capable of carrying 100 amps have been achieved. The Bi material has been produced by a powder-in-Ag-tube technique. The YBCO requires good alignment of the a-axes of the crystallites to achieve good conduction. This has been achieved by two methods: by the Rolling Assisted, Biaxially Textured (RABIT) scheme from ORNL and by Ion Beam Assisted Deposition (IBAD) of the buffer layer from LANL. Both schemes work with a flexible metal layer with buffer layer on top to provide the needed base. RABITS uses a textured metal substrate that continues the crystal orientation through the buffer layer and the applied YBCO during application. A complication is that the YBCO is only oriented for a very thin layer but inserting a Sm based layer can reset the alignment in the YBCO and thereby allow thicker oriented films with greater current carrying capability. The IBAD scheme utilizes Ar ions to orient the buffer layer system during vapor deposition and pulsed laser deposition for the YBCO layer. This high energy process requires a partial vacuum. The sense is that these technologies are advancing to where promising initial applications are feasible but that there is still plenty of room for further development.

OTHER BUSINESS

The minutes of the April 16 meeting were approved. It was determined that the election of officers would be via Email vote. The meeting was then adjourned.

CALENDAR ITEMS

Sept. 13-14, 2002:	DOE/BES Corrosion Contractors Meeting, Brookhaven National Laboratory, contact Hugh Isaacs
Sept. 17, 2002:	EMaCC meeting, Germantown, MD, contact Udaya Rao
Oct. 21-25:	Workshop on *Basic Research Needs to Assure a Secure Energy Future*, Gaithersburg, MD, contact Sharon Long
Nov. 5-6,2002:	Basic Energy Sciences Advisory Committee meeting, Gaithersburg, MD, contact Sharon Long

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The EMaCC reports to the Director of the Office of Science in his or her capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC terms of reference. This report summarizes EMaCC activities for FY 2001 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2001 was Dr. Matesh Varma. The compilation of this report was performed by Dr. Dale Koelling, EMaCC Executive Secretary for FY 2002, with the assistance of the RAND Corporation. Financial support was provided by the Industrial Materials for the Future program of the Office of Industrial Technologies and by the Office of Basic Energy Sciences.

Dr. Udaya Rao
National Energy Technology Laboratory
EMaCC Chair, FY 2002

TABLE 1
ENERGY MATERIALS COORDINATING COMMITTEE MEMBERSHIP LIST

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technology, State and Community Programs		
Building Research and Standards	Arun Vohra, EE-41	202-586-2193
Industrial Technologies		
Aluminum Vision Team	Sara Dillich, EE-22	202-586-7925
Industrial Materials for the Future	Charlie Sorrell, EE-23	202-586-1514
Transportation Technologies		
Advanced Automotive Technologies	Nancy Garland, EE-32	202-586-5673
	Joseph Carpenter, EE-32	202-586-1022
	Ray Sutula, EE-32	202-586-8064
	JoAnn Milliken, EE-32	202-586-2480
Heavy Vehicle Technologies	Sidney Diamond, EE-34	202-586-8032
Power Technologies		
Solar Energy Technologies	Richard King, EE-11	202-586-4198
Wind and Geothermal Technologies	Raymond LaSala, EE-12	202-586-1693
Hydrogen and Superconductivity Technologies	James Daley, EE-15	202-586-1165

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences and Engineering	Pat Dehmer, SC-10	301-903-3081
	Iran L. Thomas, SC-13	301-903-3427
Metals, Ceramics and Engineering	Robert J. Gottschall, SC-13	301-903-3428
	Yok Chen, SC-13	301-903-3428
	Helen Kerch, SC-13	301-903-3428
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	Richard Kelly, SC-13	301-903-3426
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Advanced Scientific Computing Research		
Technology Research	Walter M. Polansky, SC-32	301-903-5800
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Fusion Energy Sciences		
Facilities and Enabling Technologies	Sam Berk, SC-52	301-903-4171
Biological and Environmental Research		
Medical Sciences	Larry James, SC-73	301-903-7481
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Integration and Disposition		
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Science and Technology		
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NATIONAL NUCLEAR SECURITY ADMINISTRATION		
Naval Reactors	David I. Curtis, NR-1	202-781-6141
Defense Programs		
Defense Science	Bharat Agrawal, DP-133	301-903-2057
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Waste Acceptance and Transportation	Jim Carlson, RW-40	202-586-5321
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301-903-2786

ORGANIZATION OF THE REPORT

The FY 2001 budget summary for DOE Materials Activities is presented on page 9. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 11.

Following the budget summary is a set of detailed program descriptions for the FY 2001 DOE Materials activities. These descriptions are presented according to the organizational structure of the Department. A mission statement, a budget summary listing the project titles and FY 2001 funding, and detailed project summaries are presented for each Assistant Secretary office, the Office of Science, and the National Nuclear Security Administration. The project summaries also provide DOE, laboratory, academic and industrial contacts for each project, as appropriate.

FY 2001 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES

These budget numbers represent materials-related activities only. They do not include those portions of program budgets which are not materials related.

	FY 2001
OFFICE OF BUILDING TECHNOLOGIES, STATE AND COMMUNITY PROGRAMS	$1,230,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$28,629,048
Office of Industrial Strategies	11,023,000
Aluminum Vision Team	8,237,000
Forest and Paper Products Vision Team	1,050,000
Metal Casting Vision Team	1,736,000
Office of Crosscut Technologies	17,606,098
Industrial Materials for the Future (IMF) Program	12,420,000
Financial Assistance Program	5,186,048
Inventions and Innovation	2,161,819
National Industrial Competitiveness Through Energy, Environment and Economics ($NICE^3$)	3,024,229
OFFICE OF TRANSPORTATION TECHNOLOGIES	$37,985,000
Office of Advanced Automotive Technologies	23,410,000
Transportation Materials Program	19,805,000
Automotive Propulsion Materials	3,355,000
Lightweight Vehicle Materials	16,450,000
Electric Drive Vehicle Technologies	3,605,000
Advanced Battery Materials	3,605,000
Office of Heavy Vehicle Technologies	14,575,000
Heavy Vehicle Materials Technology	14,575,000
High Strength Weight Reduction Materials	8,975,000
High Temperature Materials Laboratory User Program	5,600,000
OFFICE OF POWER TECHNOLOGIES	$73,557,000
Office of Solar Energy Technologies	36,117,000
Office of Wind and Geothermal Technologies	940,000
Office of Hydrogen and Superconductivity Technologies	36,500,000
OFFICE OF SCIENCE	$551,082,034
Office of Basic Energy Sciences	501,008,000
Division of Materials Science and Engineering	501,008,000
Office of Advanced Scientific Computing Research	41,474,034
Division of Technology Research	41,474,034
Laboratory Technology Research Program	3,980,000
Small Business Innovation Research Program	36,244,071
Small Business Technology Transfer Research Program	1,249,963
Office of Fusion Energy Sciences	8,600,000

FY 2001 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (continued)

	FY 2001
OFFICE OF ENVIRONMENTAL MANAGEMENT	$3,042,996
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$15,454,365
Office of Space and Defense Power Systems	4,498,000
Space and National Security Programs	4,498,000
Office of Technology and International Cooperation	10,956,365
Nuclear Energy Plant Optimization	3,189,370
Nuclear Energy Research Initiative	7,766,995
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$113,041,000
Office of Naval Reactors	74,200,000[1]
Office of Defense Programs	38,841,000
The Weapons Research, Development and Test Program	38,841,000
Sandia National Laboratories	19,238,000
Los Alamos National Laboratory	15,330,000
Lawrence Livermore National Laboratory	4,273,000
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$30,370,100
OFFICE OF FOSSIL ENERGY	$10,568,000
Office of Advanced Research	10,568,000
Fossil Energy Advanced Research Materials Program	6,447,000
Advanced Metallurgical Processes Program	3,822,000
Ultra-Supercritical Power Plant Research	299,000
TOTAL	**$864,959,543**

[1]This excludes $50.1 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

The distribution of these funds between DOE laboratories, private industry, academia and other organizations is listed below.

TABLE 2
DISTRIBUTION OF FUNDS BY OFFICE

Office	DOE Laboratories	Private Industry	Academia	Other	Total
Office of Building Technology, State and Community Programs	$1,230,000	$0	$0	$0	$1,230,000
Office of Industrial Technologies	$7,614,500	$15,885,548	$5,129,000	$0	$28,629,048
Office of Transportation Technologies	$22,990,000	$9,635,000	$4,265,000	$1,095,000	$37,985,000
Office of Power Technologies	$45,701,000	$19,926,000	$7,930,000	$0	$73,557,000
Office of Science	$448,752,000	$37,494,034	$62,401,000	$2,435,000	$551,082,034
Office of Environmental Management	$1,665,996	$0	$1,377,000	$0	$3,042,996
Office of Nuclear Energy Science and Technology	$9,636,405	$3,299,399	$2,518,561	$0	$15,454,365
National Nuclear Security Administration	$113,041,000	$0	$0	$0	$113,041,000
Office of Civilian Radioactive Waste Management	$30,370,100	$0	$0	$0	$30,370,100
Office of Fossil Energy	$9,171,000	$524,000	$873,000	$0	$10,568,000
TOTALS	**$690,172,001**	**$86,763,981**	**$84,493,561**	**$3,530,000**	**$864,959,543**

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

The Office of Energy Efficiency and Renewable Energy seeks to develop the technology needed for the Nation to use its existing energy supplies more efficiently, and for it to adopt, on a large scale, renewable energy sources. Toward this end, the Office conducts long-term, high-risk, high-payoff R&D that will lay the groundwork for private sector action.

A number of materials R&D projects are being conducted within the Energy Efficiency and Renewable Energy program. The breadth of this work is considerable, with projects focusing on coatings and films, ceramics, solid electrolytes, elastomers and polymers, corrosion, materials characterization, transformation, superconductivity and other research areas. The level of funding indicated refers only to the component of actual materials research.

The Office of Energy Efficiency and Renewable Energy conducts materials research in the following offices and divisions:

	FY 2001
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$1,230,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$28,629,048
Office of Industrial Strategies	11,023,000
Aluminum Vision Team	8,237,000
Forest and Paper Products Vision Team	1,050,000
Metal Casting Vision Team	1,736,000
Office of Crosscut Technologies	17,606,098
Industrial Materials for the Future (IMF) Program	12,420,000
Financial Assistance Program	5,186,048
Inventions and Innovation	2,161,819
National Industrial Competitiveness Through Energy, Environment and Economic ($NICE^3$)	3,024,229
OFFICE OF TRANSPORTATION TECHNOLOGIES	$37,985,000
Office of Advanced Automotive Technologies	23,410,000
Transportation Materials Program	19,805,000
Automotive Propulsion Materials	3,355,000
Lightweight Vehicle Materials	16,450,000
Electric Drive Vehicle Technologies	3,605,000
Advanced Battery Materials	3,605,000
Office of Heavy Vehicle Technologies	14,575,000
Heavy Vehicle Materials Technology	14,575,000
High Strength Weight Reduction Materials	8,975,000
High Temperature Materials Laboratory User Program	5,600,000
OFFICE OF POWER TECHNOLOGIES	$73,557,000
Office of Solar Energy Technologies	36,117,000
Office of Wind and Geothermal Technologies	940,000
Office of Hydrogen and Superconductivity Technologies	36,500,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 2001
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS - GRAND TOTAL	$1,230,000
OFFICE OF BUILDING RESEARCH AND STANDARDS	$1,230,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,230,000
Non-HCFC Closed-Cell Foam Insulation	150,000
Insulation Materials Performance and Application	150,000
Hygrothermal Material Property Measurements and Modeling Upgrades and Applications	855,000
Sub-Ambient Pipe Insulation Materials and Systems	75,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING RESEARCH AND STANDARDS

PROGRAM GOALS

The goal of the program is to develop new building materials and building envelope systems that can contribute to the DOE energy-efficiency goal of reducing annual building energy consumption by 2 quads by year 2010 and by 5 quads by 2020, that are cost-competitive for their application and are as environmentally benign as possible.

PROGRAM OBJECTIVES

The program objectives are:

1. Search out and resolve technical issues of importance to Building America and Existing Buildings programs, the Envelope Roadmap, consumers and the buildings industry that require unique DOE research capabilities to attain DOE energy-efficiency goals;

2. Develop the scientific and engineering tools for development, demonstration and production of more energy efficient, durable, affordable, and sustainable building envelope system technologies;

3. Identify and develop new or improved insulation and other building materials;

4. Develop and standardize laboratory methods for characterizing new and existing materials;

5. Make recommendations on the effective use of building materials;

6. Develop a fundamental understanding of the physics of heat, air, and moisture flow in advanced and conventional building materials;

7. Develop and standardize field and laboratory whole envelope system performance test protocols to stimulate development and investment in energy-efficient envelope technologies;

8. Provide data developed for energy-efficient building envelope and material technologies for inclusion into the Building Codes and Standards

The DOE contact is Arun Vohra (202) 586-2193.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **NON-HCFC CLOSED-CELL FOAM INSULATION**
   $150,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Ken Wilkes (865) 574-5931

This project is for the development of foam insulations that use alternative blowing agents as drop-in replacements for the CFC blowing agents that were previously used in the manufacture of foam insulation products and for the HCFC blowing agents that are currently being used. Prototype foam insulation boards and refrigerator panels were sent to ORNL for testing and evaluation. Long-term tests are being conducted to determine thermal properties and aging characteristics. Models are being developed for aging processes, including the effects of facing materials.

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs, HCFC, Refrigerators

2. **INSULATION MATERIALS PERFORMANCE AND APPLICATION**
   $150,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Ken Wilkes (865) 574-5931

This project is for the development of accurate and reproducible data for use by the building materials community, improved test procedures to determine the thermal properties of existing, as well as advanced, insulations, interacting with the building materials research community, manufacturers, trade associations, professional societies, compliance groups and local government and making and disseminating recommendations on appropriate usage of thermal insulation to conserve energy.

Keywords: Insulation, Buildings

3. **HYGROTHERMAL PROPERTY MEASUREMENTS AND MODELING UPGRADES AND APPLICATIONS**
   $855,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Ken Wilkes (865) 574-5931

The objective of this task is to measure the hygrothermal properties of building materials that are required for modeling of moisture transport in building envelopes. Such property values are needed as inputs to moisture simulation models and provide the link between the models and large-scale experiments on moisture transfer in building envelope components. We will develop competencies that are needed to characterize the moisture control of building envelope systems. The intent of the proposed work is to develop unique hygrothermal-durability modeling capability to permit prediction long-term performance of wall systems. The model, once developed, will be used to develop guidelines for moisture management strategies for wall systems to meet user requirements of long-term performance and durability for the wide range of climate zones across North America. Properties that will be measured include sorption and suction isotherms, vapor permeance, liquid diffusivity, air permeability, specific heat and thermal conductivity. Where applicable, the properties will be measured as functions of moisture content and temperature. The laboratory will support other research on measurements and modeling of coupled heat, air and moisture transfer in building envelopes.

Keywords: Hygrothermal, Moisture, Building Materials, Heat-Air-Moisture and Properties

4. **SUB-AMBIENT PIPE INSULATION MATERIALS AND SYSTEMS**
   $75,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Bill Miller (865) 574-2013

Pipe thermal insulations are rated by the thermal resistance as measured in pipe testing apparatus in conformance with ASTM C 335. The scope of ASTM C 335 limits its use to piping systems operating at temperatures above ambient. Numerous ASTM material specifications specify the use of these materials on pipes operating below ambient conditions. There are no test methods or test facilities available for undertaking these measurements.

Pipe insulations applied to piping operating at sub-ambient conditions are also a major concern within ASHRAE. These insulation systems can have severe moisture-related problems due to the unidirectional nature of their vapor drive. Attempts to address the rash of failures to these systems due to moisture ingress leading to loss in energy efficiency as well as mechanical failure are planned.

Keywords: Piping, Moisture, Insulation and Properties

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 2001
OFFICE OF INDUSTRIAL TECHNOLOGIES - GRAND TOTAL	$28,629,048
OFFICE OF INDUSTRIAL STRATEGIES	$11,023,000
ALUMINUM VISION TEAM	$8,237,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$5,032,000
Innovative Vertical Floatation Melter (VFM)	400,000
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	500,000
Intelligent Potroom Operation	428,000
Development of a Novel Non-consumable Anode for Electrowinning Primary Aluminum	381,000
Potlining Additives	493,000
Reduction of Oxidative Melt Loss of Aluminum	745,000
Selective Adsorption of Salts from Molten Aluminum	55,000
Aluminum Carbothermic Technology	1,107,000
Wetted Cathodes for Low Temperature Smelting	452,000
High Efficiency Low Dross Combustion System	371,000
A Bubble Probe for Optimization of Bubble Distribution and Minimization of Splashing/Droplet Formation	100,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,161,000
Semi Solid Aluminum Alloys	260,000
Integrated Numerical Methods and Design Provisions for Aluminum Structures	93,000
Textures in Aluminum Alloys	308,000
Reduction of Annealing Times for Energy Conservation in Aluminum Processing	100,000
Surface Behavior of Aluminum Alloys Deformed under Various Processing Conditions	100,000
Fundamental Studies of Structural Factors Affecting the Formability of Continuous Cast Aluminum Alloys	100,000
Development of a Two-phase Model for the Hot Deformation of Highly-Alloyed Aluminum	100,000
Development of Integrated Methodology for Thermo-mechanical Processing of Aluminum Alloys	100,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,044,000
Recycling Aluminum Salt Cake	300,000
Processing and Recycling of Aluminum Wastes	111,000
Wettable Ceramic-based Drained Cathode Technology for Aluminum Electrolysis Cells	720,000
Spray Rolling Aluminum Strip	269,000
Modeling Optimization of Direct Chill Casting	644,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2001
OFFICE OF INDUSTRIAL STRATEGIES (continued)	
FOREST AND PAPER PRODUCTS VISION TEAM	$1,050,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING	$1,050,000
Corrosion in Kraft Digesters: Characterization of Degradation and Evaluation of Corrosion Control Methods	750,000
Selection and Development of Refractory Structural Materials for Black Liquor Gasification	300,000
METAL CASTING VISION TEAM	$1,736,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$373,000
Creep Resistant Zinc Alloy Development	132,000
Development of Surface Engineered Coatings for Die Casting Dies	149,000
Integration of RSP Tooling with Rapid Prototyping for Die-Casting Application	92,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING	$1,363,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	332,000
Prevention of Porosity in Iron Castings	45,000
Advanced Lost Foam Casting Technology	325,000
Metallic Reinforcement of Direct Squeeze Die Cast Aluminum Alloys	100,000
Ferrite Measurements in Duplex Stainless Steel Castings	70,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	215,000
Improvements in Sand Mold/Core Technology: Effects on Casting Finish	176,000
Heat Checking and Washout of Superalloys for Die Inserts	100,000
OFFICE OF CROSSCUT TECHNOLOGIES	$17,606,048
INDUSTRIAL MATERIALS FOR THE FUTURE (IMF) PROGRAM	$12,420,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$3,490,000
Advanced Materials/Processes	1,090,000
Composites and Coatings Through Reactive Metal Infiltration	300,000
Conducting Polymers: Synthesis and Industrial Applications	150,000
Development of Advanced Metallic/Intermetallic Alloys	670,000
High Temperature Facilitated Membranes	300,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	680,000
Plasma Processing-Advanced Materials for Corrosion and Erosion Resistance	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,680,000
Continuous Fiber Ceramic Composites (CFCC) - Supporting Technologies	1,150,000
Materials Development for the Forest Products Industry	980,000
Metals Processing Laboratory Users (MPLUS) Facility	550,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2001
OFFICE OF CROSSCUT TECHNOLOGIES (continued)	
INDUSTRIAL MATERIALS FOR THE FUTURE (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,750,000
Continuous Fiber Ceramic Composites (CFCC) - Industrial Technologies	1,500,000
Selective Inorganic Thin Films	250,000
INDUSTRIES OF THE FUTURE MATERIALS ISSUES	$4,500,000
IMF Call for Proposals for 2001	4,500,000
FINANCIAL ASSISTANCE PROGRAM	$5,186,048
INVENTIONS AND INNOVATION	$2,161,819
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,161,819
Laser Sensor For Optimization of Compressor Stations and Refinery Operations	0[1]
Titanium Matrix Composite Tooling Material for Enhanced Manufacture of Aluminum Die Castings	0[1]
An Insoluble Titanium-lead Anode for Sulfate Electrolytes	0[1]
Development of an Innovative Energy Efficient High Temperature Natural Gas Fired Furnace	0[1]
A New High Temperature Coating for Gas Turbines	0[1]
Tough-coated Hard Powders (TCHPS): a New Paradigm in Mining and Machining Tool Materials	0[1]
A New Energy Saving Method of Manufacturing Ceramic Products from Waste Glass	0[1]
Distillation Column Flooding Predictor	0[1]
Energy Saving Lightweight Refractory	0[1]
High Intensity Silicon Vertical Multi-junction Solar Cells	0[1]
Fabrication And Testing of a Prototype Ceramic Furnace Coil	0[1]
Germanium Compounds as Highly Selective Fluorination Catalysts	0[1]
Development of Phosphors for Use in High-efficiency Lighting and Displays	0[1]
Novel Ceramic Composition for Hall-Heroult Cell Anode Application	0[1]
Functionally Graded Materials for Improved High Temperature Performance of Nd-Fe-B-based Permanent Magnets	0[1]
Improved Alkylation Contactor	0[1]
Low Cost Synthesis and Consolidation of TiC	0[1]
Development of Aluminum Iron Alloys for Magnetic Applications	0[1]
Novel Frequency-Selective Solar Glazing System	0[1]
A Ceramic Composite for Metal Casting	0[1]
Electrochemical Method for Extraction of Oxygen from Air	0[1]
Energy Saving Method for Producing Ethylene Glycol and Propylene Glycol	0[1]
Improved Refractories Using Engineered Particles	0[1]
Enabling Tool for Innovative Glass Applications	0[1]
Distributed Optical Sensors for Continuous Liquid Level Tank Gauging	0[1]

[1]Prior Year Funding

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

OFFICE OF CROSSCUT TECHNOLOGIES (continued)

FINANCIAL ASSISTANCE PROGRAM (continued)

INVENTIONS AND INNOVATION (continued)

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)

	FY 2001
A Low Energy Alternative to Commercial Silica-based Glass Fibers	0[1]
Cromer Cycle Air Conditioning	0[1]
A Viable Inert Cathode for Smelting Primary Aluminum	40,000
Development of Inert Anode for the Primary Aluminum Industry	40,000
Catalytic Processors for CO_2 Reforming of CH_4 and Gaseous Hydrocarbons	40,000
Testing a Highly Efficient Technology for Converting Woody Biomass to Electricity	40,000
Automatic Evaluation of Wood Properties	39,896
Improved Process Control of Wood Waste Fired Boilers	40,000
Energy-efficient Production and Utilization of Light-weight Structural Panels	40,000
High Purity Fused Silica Glasses	40,000
Batch Preheat for Glass and Related Furnace Processing Operations	40,000
Development of Environmentally Benign Mineral Flotation Collectors	40,000
A Microbial Genomics Approach to Resource Exploration and Characterization	40,000
New Membrane Process for Improved Energy Saving Separations in the Petroleum Industry	40,000
Coke Formation Process Model for Petroleum Refining Efficiency Improvement	39,519
Fluted Spiral Membrane Module for Reverse Osmosis of Liquids with Dissolved and Suspended Solids	40,000
Electrochromic Window Film	40,000
Process Particle Counter (PPC) Sensor/Controller for Optimizing Power Recovery Expander and Gas Turbine Performance for Various Fuel Sources	106,942
Thermophotovoltaic Electric Power Generation Using Exhaust Heat in the Glass, Steel and Metal-casting Industries	199,806
Lost Foam Casting Quantifier Program	64,042
A Hot Eye™ Based Coordinate Measuring Machine for the Forging Industry	130,226
Development of a High-frequency Eddy-current Separator	126,942
Integrated Acoustic Kiln Monitor to Guide Accelerated Drying of Wood	91,942
Development of an Energy-Saving Grain Drying Invention	41,942
System for Detection and Control of Deposition in Kraft Recovery Boilers and Monitoring Glass Furnaces	83,942
Development and Commercialization of Biopulping	174,942
Development of a Lower pH Copper Flotation Reagent System	91,692
Miniature, Inexpensive, Amperometric Oxygen Sensor	126,942
Extremely Compact and Efficient Chemical Reactor	139,942
High Throughput Vacuum Processing for Innovative Uses of Glass	76,942
Energy Conservation Waste Reduction in the Processing of Soft (Unfired) Ceramic Particles via Dynamic Cyclone Classification	106,160

[1]Prior Year Funding

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2001
OFFICE OF CROSSCUT TECHNOLOGIES (continued)	
FINANCIAL ASSISTANCE PROGRAM (continued)	
NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE[3])	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,024,229
Demonstration of a Three-phase Rotary Separator Turbine	0[1]
Precision Irrigation Technologies for the Agricultural Industry	0[1]
Energy Conserving Tool for Combustion Dependent Industries	0[1]
Energy-saving Regeneration of Hydrochloric Acid Pickling Liquor	0[1]
Supercritical Fluid Purification of Combi-chem Libraries	0[1]
Full-scale 100 Ton/hr Demonstration of Magnetic Elutriation Technology for Clean And Efficient Processing of Iron Ore	0[1]
Production-scale Commercial Demonstration of a Vanadium Carbide Coating Process for Enhancing Wear Resistance of Metals in Steel and Other Manufacturing Industries	491,840
Commercial Demonstration of an Improved Magnesium Thixomolding Process	484,000
Improvement of the Lost Foam Casting Process	525,000
Support Inspection: a Method of Inspecting On-stream Process Piping at Support Areas	474,994
The Flex-microturbine for Pecan Waste: Electricity and Heat in a Nutshell	523,395
Pressurized Ozone Membrane Ultrafiltration Methodology for TDS Removal in Paper Mill Process Water for Energy Savings, Production Efficiency, and Environmental Benefits	525,000

[1]Prior Year Funding

OFFICE OF INDUSTRIAL TECHNOLOGIES

OFFICE OF INDUSTRIAL STRATEGIES

ALUMINUM VISION TEAM
The DOE Aluminum Team leader is Sara Dillich
(202) 586-7925

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

5. **INNOVATIVE VERTICAL FLOATATION MELTER (VFM)**
$400,000
DOE Contact: Ramesh Jain (202) 586-2381

The Energy Research Company, O'Brien & Gere Engineers, Inc., and Stein, Atkinson Stordy Ltd. are project partners for the development of VFM. Recycled aluminum accounts for more than one third of the total U.S. aluminum supply. Aluminum recycling results in significant energy savings, lower emissions and an increase in metal yield. Typically, aluminum scrap is cleaned/decoated and then melted in gas reverberatory furnaces that have low thermal efficiencies (20 percent) and generate substantial emissions. The vertical floatation melter is an innovative design that decoats, preheats and melts in one operation. The pilot demonstrated design provides a thermal efficiency of 58 percent. Not only is energy saved, but also the emissions are significantly reduced and more metal is recovered. The design provides a higher metal yield (dross reduction) because of lower gas temperature, lower residence time, lower oxygen content and no direct flame impingement on the metal. The VFM is a versatile design that can be integrated with indirect-fired controlled-atmosphere rotating kilns. This integration provides additional savings, with thermal efficiencies of over 75 percent in recovering aluminum scrap. This process also has applications in the glass and steel industries. A pilot scale unit capable of processing 1,000 pounds per hour of aluminum has been designed, constructed and successfully tested. Pilot operations have demonstrated a thermal efficiency (the ratio of heat going into scrap aluminum to that of the total energy used) of more than 2.5 times that of a conventional furnace, lower emissions and improved metal recovery (dross reduced by more than half). This project has now entered the planning, site preparation and field-testing phase that will demonstrate the VFM's commercial use.

Keywords: Floatation Melter, Aluminum Scrap

6. **INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS**
$500,000
DOE Contact: Simon Friedrich (202) 586-6759

Northwest Aluminum Technologies and Brooks Rand, Ltd. are project partners for the development of this technology. A carbon-free aluminum reduction process is being developed as a modification to the Hall-Héroult process for primary aluminum production. The process uses a non-consumable metal alloy anode, a wetted cathode, and an electrolytic bath, which is kept saturated with alumina at the relatively low temperature of 750°C by means of free alumina particles suspended in the bath. In conducting the research, two primary tasks are involved. First, laboratory scale cells will be operated to firmly establish the viability of the fundamental concepts required for a successful commercial process. Second, a pilot scale 5000-ampere cell will be designed, constructed and operated. This task will address engineering aspects associated with scaling, such as liner fabrication, electrode configuration and design, and bath composition adjustments. This technology, once developed, will produce primary aluminum metal with lower energy intensity, lower cost, and lower environmental degradation than the conventional process.

Keywords: Aluminum Reduction, Inert Metal Anode, Smelting, Alumina Crucible Cell, Voltage

7. **INTELLIGENT POTROOM OPERATION**
$428,000
DOE Contact: Simon Friedrich (202) 586-6759

Applied Industrial Solutions, Century Aluminum, and West Virginia University are project partners for the development of intelligent potroom operation. Aluminum smelting requires operators to oversee many refining cells. Scrutiny of each one on a regular basis is not possible. In addition, modern aluminum refining cell controllers attempt to optimize cell efficiency by controlling the concentration of alumina in the bath. Unfortunately, no direct measure of alumina concentration is yet possible. The ramifications miscalculating alumina concentration is significant from an environmental and energy efficiency standpoint. One major product of this research will be the development of a Corrective Action Neural Network (CANN). Its function is to monitor and analyze data from the pots on a continuous basis, looking for cells whose performance is deteriorating. It will anticipate which cells are about to slip into degraded or out-of-control operation and dispatch the operator to intervene before trouble begins. Eventually, a closed-loop Cell Control Enhancement Module (CCEM) will be added to the individual cell controllers. The CCEM will use an enhanced instrumentation package and powerful data analysis techniques to provide a more complete picture of instantaneous cell status to the CANN. The CANN and CCEM will work in concert to continuously improve the database on each cell, and the knowledge base on control and remediation techniques.

Keywords: Smelting, Aluminum Potroom Operation, Aluminum Refining

8. **DEVELOPMENT OF A NOVEL NON-CONSUMABLE ANODE FOR ELECTROWINNING PRIMARY ALUMINUM**
$381,000
DOE Contact: Simon Friedrich (202) 586-6759

Ohio State University assisted by Gas Research Institute, Kaiser Aluminum, Siemens-Westinghouse and TDA Research are project partners for the development of a novel non-consumable anode. Since the patenting of the Hall-Héroult Cell (HHC) in 1886 for electrowinning aluminum, the basic features have remained essentially the same. Although significant optimization has occurred, industry acknowledges that there are many problems associated with the use of the consumable carbon anode. This project is developing a novel non-consumable (gas) anode that will displace today's carbon anode (eliminating the carbon plant), and serve as a retrofit into the current HHC. The anode is comprised of a thin, dense oxide-ion-conducting membrane with an electrocatalytic porous internal anode where reformed natural gas is electrochemically oxidized. Application of such a non-consumable anode retrofitted into the HHC would significantly increase the energy efficiency, reduce the emissions, and reduce the cost of producing primary aluminum compared to the best current and emerging anode replacement technologies.

Keywords: Carbon Anode, Aluminum Production, Smelting

9. **POTLINING ADDITIVES**
$493,000
DOE Contact: Simon Friedrich (202) 586-6759

This project is designed to further examine the potential benefits derived from the addition of boron oxide to potlining used in primary aluminum production cells. A relatively inexpensive bulk chemical, boron oxide not only suppresses cyanide formation, but also may inhibit sodium intercalation and, above all, promote, in the presence of some titanium, wetting of cathode carbonaceous material by the metal pad, thus reducing ohmic cell resistance and sludge formation. Improvements in energy consumption, waste disposal and overall economics of the process are projected. Laboratory testing and commercial scale testing will investigate parameters that are important for the commercial application. Tests in industrial cells will complement laboratory testing. Carbonaceous potlining components added with boron oxide will be incorporated in industrial cells in later phases of the program, providing results of the first year are positive. Project partners include Century Aluminum of West Virginia, Inc., EMEC Consultants, the NSA Division of Southwire Company and SGL Carbon Corporation.

Keywords: Potlining, Smelting, Aluminum Production, Boron Oxide, Aluminum Production Cells

10. **REDUCTION OF OXIDATIVE MELT LOSS OF ALUMINUM**
$745,000
DOE Contact: Simon Friedrich (202) 586-6759

Fabrication of virtually all finished aluminum products requires melting. During the melting process, an average of 4 percent of the input material is lost to oxidation. The lost material takes three forms in the furnace: 1) dross, a mixture of aluminum oxide compounds and aluminum metal typically skimmed from the surface of the melt; 2) inclusions entrained in the molten metal removed by filtration; and 3) oxide sludge found at the bottom of the melt. In the U.S., an annual energy loss of approximately 70 trillion Btu results from oxidative melt loss of over 960 million pounds of aluminum. This project will target practices to significantly reduce these losses. The melt loss project will identify aluminum melting practices that will increase energy efficiency and decrease material losses. The project will lower the cost of aluminum products, reduce energy consumption, reduce industrial emissions, and significantly increase the recycling capability of the aluminum industry. An increased fundamental understanding of the oxidation of molten aluminum will be developed to be a cross-section of the aluminum industry. Project partners include Secat, Inc., Commonwealth Aluminum, Hydro Aluminum, IMCO Recycling Inc., NSA Division of Southwire Co., Alcan Aluminum Corp., ARCO Aluminum Inc., McCook Metals LLC, Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Dross, Aluminum Melting, Oxide Sludge

11. **SELECTIVE ADSORPTION OF SALTS FROM MOLTEN ALUMINUM**
$55,000
DOE Contact: Simon Friedrich (202) 586-6759

Selee Corp. and Alcoa are project partners for the development of this Selective Adsorption technology. Primary aluminum is produced by the reduction of alumina in electrolytic cells. Cells contain a molten cryolite bath in which the alumina is dissolved. When an electric current is applied, aluminum is released and settles to the bottom of the cell. Molten aluminum is withdrawn to holding furnaces, and alumina is added to the bath as it is consumed. In normal production, a small portion of the bath is carried over with the molten aluminum. Most of the bath carry-over can be removed by careful skimming and good transfer practices. However, some carry-over of the bath to the metal holding furnace is common. Cryolite bath contains sodium and small amounts of calcium and lithium. These metal salts must be removed from aluminum in the holding furnace to produce metal of commercial value. Chlorine is used to remove these salts. Bath carry-over is undesirable because it adds significantly to the time required and the amount of chlorine used to make commercial aluminum. A new microporous material has been demonstrated to selectively adsorb salts from molten aluminum in holding furnace operations. This project will evaluate the potential of adapting these microporous materials to remove carry-over salts. Successful removal of these salts will result in significant reductions of energy, chlorine and metal loss.

Keywords: Alumina, Microporous Materials, Cryolite, Primary Aluminum

12. **ALUMINUM CARBOTHERMIC TECHNOLOGY**
$1,107,000
DOE Contact: Simon Friedrich (202) 586-6759

Alcoa Technical Center, Elkem Aluminum Division, and Carnegie Mellon University are project partners for the development of the advanced reactor process (ARP). ARP is a new process for the production of aluminum by carbothermic reduction. This technology has been proposed as an alternative to the current Hall-Héroult electrolytic reduction process. ARP has the potential to produce primary aluminum at a power consumption in the range of 8.5 kWh/kg at an estimated 25 percent reduction in manufacturing cost. Although the carbothermic process involves the generation of carbon-based greenhouse gases (GHG), the total GHG reduction from power plant to metal should be substantial due to the significantly reduced power consumption, the elimination of perfluorocarbon emissions, and the elimination of carbon anode baking furnace emissions. The estimated capital investment required for ARP will be about 50 percent less than that for Hall-Héroult cell technology. The labor required for plant operation will also be reduced. ARP is a multi-step high temperature chemical reaction that produces aluminum by reduction of alumina with carbon. Optimization for reaction products requires a multi-zone furnace operating at temperatures in excess of 2,000˚C. A significant portion of the aluminum is in the gas phase at these temperatures. A continuously operating furnace capable of producing the high temperatures required and recovering the molten and gas phase products is critical for the development of this technology. This is Phase I of a multi-phase effort to develop an ACT reactor based on advanced, high temperature, electric-arc furnace technology and improved understanding of the process reactions.

Keywords: Aluminum Carbothermic Reduction, Advanced Reactor Process, Alumina

13. **WETTED CATHODES FOR LOW TEMPERATURE SMELTING**
$452,000
DOE Contact: Simon Friedrich (202) 586-6759

Wetted cathodes and inert anodes have potentially significant advantages over the century old Hall-Héroult cell used today for worldwide aluminum production. Wetted cathodes allow for decreased anode-cathode distances accompanied by reduced voltages and energy consumption. Inert anode replacement of conventional carbon anodes will eliminate the emission of greenhouse gases associated with the production of primary aluminum (e.g., CO, CO_2 and perfluorocarbons) and with the manufacture of the carbon anodes. The use of wettable cathodes with inert anodes could reduce the energy needed for primary aluminum production by 25 to 30 percent. The adoption of these advanced electrodes has been hindered by their rapid corrosion, particularly of the cathode, when operating at a conventional temperature of 950˚C. A low temperature electrolysis (LTE) cell that operates about 200˚C lower than a conventional cell offers a more benign environment for advanced electrodes. This project will extend the knowledge of wetted cathode operation and failure mechanisms. It will prepare and screen various wetted cathode materials for aluminum LTE cells and develop techniques to measure and evaluate the aluminum film on the wetted cathode. Successful development of this technology will lower both capital and operating costs and offer many advantages in energy and environmental conservation. Project partners include Northwest Aluminum Technologies, assisted by Advanced Refractory Technologies, Material Modification Inc., Electrochemical Technology Corp., Brooks Rand Limited, and Pacific Northwest National Laboratory.

Keywords: Low Temperature Electrolysis, Inert Anode, Wetted Cathode

14. **HIGH EFFICIENCY LOW DROSS COMBUSTION SYSTEM**
$371,000
DOE Contact: Simon Friedrich (202) 586-6759

Over 70 percent of 2.3 million tons of secondary aluminum recovered from scrap is processed in reverberatory furnaces. These furnaces are widely used because of their versatility and low capital cost. Despite their benefits, reverberatory furnaces exhibit uneven surface temperature and exposure to oxygen that promotes the production of dross on the surface of the molten aluminum. Dross formation lowers aluminum productivity and insulates the molten aluminum thereby lowering energy efficiency. This project will develop and demonstrate a high-efficiency low-dross combustion system for secondary aluminum natural gas-fired reverberatory furnaces. Oxygen enrichment is key to improving burner efficiency and has been demonstrated in many industries. Oxygen enriched flames are hotter than air-fired flames and can promote dross formation. However, new burners and controls allow for the control of the flame shape and distribution of oxygen within the flame. Controlling the flame with a fuel rich zone on the flame bottom ensures that the molten aluminum has minimal exposure to oxygen and minimizes dross formation. At the same time, control of the flame shape ensures that the surface is evenly heated. Upon successful completion, this project will decrease energy requirements, improve economics, and decrease gaseous and solid emissions from the remelting of aluminum. This technology can also be retrofitted to existing reverberatory furnaces. Project partners include Gas Technology Institute, assisted by Wabash Alloys, LLC, Eclipse Combustion Inc., and University of Illinois Chicago.

Keywords: Reverberatory Furnace, Low-Dross Combustion, Secondary Aluminum

15. **A BUBBLE PROBE FOR OPTIMIZATION OF BUBBLE DISTRIBUTION AND MINIMIZATION OF SPLASHING/ DROPLET FORMATION**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

Primary and secondary aluminum producers and foundries remove impurities from molten aluminum by bubbling chlorine through the molten metal as a reactive fluxing gas. An example of chlorine fluxing is the removal of magnesium from close to 64 billion recycled aluminum cans (2 billion pounds of aluminum) to match the high purity that is representative of aluminum produced from electrolytic cells. Primary aluminum producers also use gas fluxing to remove trace alkali metals from the electrolyte present in the electrolytic cells. However, fluxing yields toxic gases such as hydrogen chloride and chlorine as well as aluminum oxide fumes. Chlorine bubbling is poorly controlled. Excess chlorine is used to ensure impurities are reduced to acceptable levels, which results in both the loss of aluminum (AlCl3) and the emission of oxide fumes and toxic gases. Optimizing fluxing gas bubble size, frequency and residence time, and understanding how gas throughput may be increased without splashing and spraying of molten metal as the bubbles burst at surface would substantially reduce chlorine usage, increase productivity and thermal efficiency of aluminum purification process, and reduce toxic gas emissions. Project partners include University of California, Berkeley, assisted by Alcoa Technical Center.

Keywords: Gas Fluxing, Chlorine, Primary Aluminum

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

16. **SEMI SOLID ALUMINUM ALLOYS**
$260,000
DOE Contact: Simon Friedrich (202) 586-6759

Semi-solid material processing offers distinct advantages over other near-net-shape manufacturing processes. In this process, cast parts are produced from slurry kept at a temperature between the solidus and the liquidus isotherms. This process produces complex parts with better quality when compared to parts made by similar processes. It also allows net-shape forming, reducing further machining operations. The process combines the advantages of both liquid metal casting and solid metal forging. The purpose of this project is to achieve a better understanding of the fundamental issues concerning the constitutive behavior of semi-solid materials and their behavior during processing, so that the applicability of semi-solid forming can be extended to various aluminum alloy systems. Worcester Polytechnic Institute (WPI) will be using numerical simulations to predict die filling and, ultimately, die design optimization. A Herschel-Bulkley fluid model, modified to account for the two-phase nature and time-dependent rheological behavior of SSM slurries, will be used with specially developed computational codes for semi-solid fluid flow and die filling to produce simulations for the filling of two-dimensional and three-dimensional cavities under various processing conditions. Issues related to die design and temperature control would also be addressed using numerical simulations. The Massachusetts Institute of Technology work will concentrate on obtaining fundamental rheological data needed for the WPI modeling and simulation activity. MIT will determine effects of semi-solid slurry structure on flow behavior and flow separation at high shear rates representative of actual forming processes. The work at Oak Ridge National Laboratory will concentrate on characterizing the thermophysical properties of semi-solid aluminum alloys and the development of new optimally designed alloys.

Keywords: Semi-Solid Forming, Aluminum Alloys, Net-Shape Forming

17. **INTEGRATED NUMERICAL METHODS AND DESIGN PROVISIONS FOR ALUMINUM STRUCTURES**
$93,000
DOE Contact: Simon Friedrich (202) 586-6759

Project partners for this research effort are the Aluminum Association and Cornell University. Aluminum's competitive edge arises from the ease with which shapes can be extruded. Yet, this advantage cannot be fully exploited by designers because they do not have the tools to predict the strength of many extrudable shapes. Suggested specifications for the structural design of parts made of various aluminum alloys were developed in 1962 and published in 1967 in Specifications for Aluminum Structures (Aluminum Association). The document has been revised five times, most recently in 1994, but methods for determining the buckling strength of extrusions are essentially unchanged. Many types of stiffeners, such as web stiffeners and multiple intermediate stiffeners, thickness changes and other cross-sectional peculiarities cannot be addressed by the current specification even though they add significantly to the load carrying capacity. Researchers from Cornell University will develop and demonstrate a design methodology using finite strip analysis. It will result in design rules applicable to many extrudable or cold-rolled shapes. Columns, beams, and beam columns will be studied. A wide variety of failure modes such as local, distortional, torsional, torsional-flexural, and lateral buckling will be researched. Failures involving the interaction of these modes, such as the local and overall buckling will be included in the study as well.

Keywords: Aluminum Extrusions, Aluminum Structures, Design Provisions

18. **TEXTURES IN ALUMINUM ALLOYS**
$308,000
DOE Contact: Simon Friedrich (202) 586-6759

Aluminum sheets made by continuous strip casting provide energy savings of greater than 26 percent and cost savings of more than 19 percent compared to sheets made from ingot casting and rolling. Sheet formability is among the most important characteristics of aluminum sheet. Formability depends on the crystal grain structure and is a result of the casting method and processing sequences used to produce the sheet. The demand for aluminum sheets is increasing particularly in the transportation industry where they are used to produce lighter, more fuel-efficient vehicles. As more complex forms are required, improved process controls are needed. Industry currently relies on post-processing testing to determine formability characteristics of finished sheet. The on-line monitoring of the continuously cast sheet production process will allow simultaneous control of important forming parameters. Crystallographic texture is related to the mechanical anisotropy/formability of metallic sheets. University of Kentucky and Commonwealth Aluminum will determine if there is a quantitative relationship between crystallographic texture measurements at processing temperatures and aluminum sheet formability. Data will be collected from two different spectroscopic measuring devices. This data will then be analyzed to determine if these instruments can produce measurements of the formability characteristics. The instrument proven to be most effective for measuring texture and formability at processing temperatures will be installed on-line in a production facility to demonstrate the ability to measure and control formability in continuous strip production.

Keywords: Textures in Aluminum Alloys, Crystallographic, Continuous Casting

19. **REDUCTION OF ANNEALING TIMES FOR ENERGY CONSERVATION IN ALUMINUM PROCESSING**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

Annealing processes in the early stages of aluminum processing affect the structure and properties of the material. A necessary step in processing all direct chill ingots is breakdown and hot rolling. In the typical single-stand mill, the time, temperature and deformation experienced by material varies considerably and is highly variable with respect to location along the workpiece and across the section. Several large-volume, non-heat treatable aluminum alloys require one or more annealing steps in order to recrystallize the material. Recrystallization requires long-range motion of grain boundaries to restore the mechanical state ready for further processing, or sale to customer. Although recrystallization is a well understood process, very little is known in a quantitatively about the influence of impurities and crystallography on the critical process. The focus of this research will be to measure these effects, relate them to the actual compositions and deformation processing of real alloys and seek to minimize annealing times. Project partners will research how the annealing processes in early stages of aluminum processing affect the structure and properties of the material. Annealing at high temperatures consume significant amounts of time and energy. By making detailed measurements of the crystallography and morphology of internal structural changes, they expect to shorten processing times and use less energy during annealing while improving texture control in production of plate and sheet through a study of the kinetics of recrystallization in hot rolling. The research will exploit newly developed tools for textural and microstructural characterization to measure recrystallization kinetics and texture evolution. Project partners include Carnegie Mellon University, assisted by Alcoa Technical Center and the Pennsylvania Technology Investment Authority.

Keywords: Annealing, Recrystallization, Hot Rolling

20. **SURFACE BEHAVIOR OF ALUMINUM ALLOYS DEFORMED UNDER VARIOUS PROCESSING CONDITIONS**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

Lehigh University and Alcoa Technology are project partners for establishing a relationship between surface behavior, metallurgy, and mechanical forming process parameters. Research will determine the fundamentals controlling surface microstructure development for rolling and extrusion processes. The objective is to understand the origins and mechanisms of the formation of surface phenomena including surface re-crystallization and surface fracture. Understanding the origins and mechanisms that control surface quality in formed aluminum products can help industry to reduce scrap, improve process efficiency, lower production costs, and save energy. Formed products are produced by complex thermo-mechanical deformation operations such as rolling and extrusion. These metal-forming operations can create surface flaws which affect surface anodizing and coating. Demand is rapidly growing for high quality formed aluminum products in the automotive and aerospace industries. Surface quality is part of the formed aluminum product specifications and is of comparable importance to mechanical properties and alloy composition.

Keywords: Surface Behavior, Metallurgy, Aluminum Alloys

21. **FUNDAMENTAL STUDIES OF STRUCTURAL FACTORS AFFECTING THE FORMABILITY OF CONTINUOUS CAST ALUMINUM ALLOYS**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

University of Kentucky is collaborating with Commonwealth Aluminum Company, Oak Ridge National Laboratory, and Secat, Incorporated in conducting these studies. Aluminum sheets made by continuous casting (CC) provide an energy savings of at least 25 percent and an economic savings of more than 14 percent over sheets made from direct chill (DC) cast ingots. Width and formability are among the most important characteristics of aluminum sheets. There are substantial differences in the microstructures of CC and DC cast sheets that are a result of the casting process. Understanding the microstructure differences and how these relate to product forming is required before industry will invest the large capital required for wide continuous cast sheet equipment. The ability to continuously cast wide sheets with good formability microstructure will make the energy and economic savings available to a greater portion of the sheet forming market. The research will focus on determining the influence of the cast microstructure and the spatial distribution of the intermetallic constituents and dispersion phases of the microtexture during deformation and recrystallization. The object of this research is to study in detail the difference in structure between DC and CC aluminum alloys that leads to the difference in formability. This work will concentrate on the 5000 series aluminum alloys, which have great potential for continuous cast product market growth. The difference in formability will be correlated with the difference in bulk texture and microtexture of the two materials. The fundamental insight obtained from this research will provide a science-based approach for optimizing wide continuous casting technology.

Keywords: Continuous Casting, Microtexture, Direct Chill Casting

22. **DEVELOPMENT OF A TWO-PHASE MODEL FOR THE HOT DEFORMATION OF HIGHLY-ALLOYED ALUMINUM**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

Conventional processing methods for highly alloyed aluminum consist of ingot casting, followed by hot rolling. These alloys are susceptible to the development of defects in hot rolling, due to localized melting along the chemistry rich grain boundaries. Much energy is wasted through the need to re-melt and reprocess. For both conventional hot rolling an novel processes such as continuous casting, quality will be achieved only through understanding of the flow of the alloyed aluminum at temperatures approaching the melting point. The research partners; University of Illinois, Alcoa, and Los Alamos National Laboratory, are developing a fundamental understanding for deformation of wrought alloys with emphasis on high temperatures bounding the hot working regime. Traditional constitutive models consider the alloy as a single-phase system. This research is offering a plan that spans the identification of fundamental deformation mechanisms using high-resolution electron microscopy and actualization into modeling capability appropriate for industrial processes. This research is developing a two-phase mathematical description for the high temperature flow of aluminum alloys. The focus is on hot rolling and provides a computation platform for optimization of the Thermo-mechanical processing window (TPW) within industrial capabilities of temperature and deformation rate. The key research challenge is the formulation of robust relations that detail mechanical behavior in the presence of a semi-solid phase. Success in the research effort and subsequent implementation in the domestic aluminum industry would provide an energy savings, a carbon dioxide reduction, a cost savings to the U.S. aluminum industry, and a reduction in scrap.

Keywords: Ingot Casting, Hot Rolling, Aluminum Alloys

23. **DEVELOPMENT OF INTEGRATED METHODOLOGY FOR THERMO-MECHANICAL PROCESSING OF ALUMINUM ALLOYS**
$100,000
DOE Contact: Simon Friedrich (202) 586-6759

Washington State University, Alcoa Technology, and

Pacific Northwest National Laboratory are project partners for the development of the integrated methodology for thermomechanical processing of aluminum alloys. The objective of this research is to develop an integrated methodology for modeling local structural evolution during thermomechanical processing (TMP) of rolled aluminum sheet for alloy design and manufacturing. Current alloys and processes are over-engineered at a substantial energy and material cost to aluminum producers. Better understanding of the physics of deformation and structure development will result in the opportunity to reduce alloy content, minimize processing steps, and improve performance of existing products. This research will involve developing a finite element based integrated mechanical and micro-structural model for process understanding and design sensitivity analyses and validating the integrated model predictions through bench-scale experimental measurements. The ultimate goal is to produce models that will allow simultaneous process modeling and alloy development. The integrated model will enable researchers to simultaneously address both materials dynamics and mechanical behavior for alloy design and for thermomechanical process optimization. The end-result will be processes optimized to reduce or eliminate energy intensive batch anneals during processing of automotive sheet. The integrated model will involve both local scale simulation of dislocation dynamics and microstructure evolution and macro-scale mechanical deformation simulations. The fundamental understanding and technology improvements derived from this research will translate into significant energy savings and great financial and environmental benefits to the aluminum industry.

Keywords: Thermomechanical Processing, Advanced Reactor Process, Alloys

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

24. **RECYCLING ALUMINUM SALT CAKE**
$300,000
DOE Contact: Simon Friedrich (202) 586-6759
ANL Contact: John Hryn (630) 252-5894

Salt cake recovery is the most energy and cost intensive unit operation in the recovery of salt cake constituents. In this project, Argonne National Laboratory (ANL) is developing a salt recovery process based on electro-dialysis (ED). Laboratory scale experiments and economic analysis has indicated that, for conditions consistent with salt cake recycling, the ED technology is more cost-effective for salt recovery than alternative technologies (e.g., evaporation with vapor recom-pression). Increasing the market value of non-metallic product (NMP) is critical for cost-effective salt cake recycling. Impurities constitute about 10 percent of NMP and lower its market value. Research investigated hydrometallurgical processes to purify NMP, since higher NMP purity results in higher market value for refractory aggregate and other potential alumina markets. Technical and economic analysis indicated the electrodialysis process to be most promising. Pilot-scale work indicated fiber insulation materials can be made cost-effectively using NMP as a starting material. A new potential use for NMP (i.e. as alternative alumina units for the blast furnace in ironmaking) has been identified. Process flow sheet and engineering design for pilot scale testing of the electrodialysis process have been completed.

Keywords: Aluminum, Salt Cake, Recycling, Electrodialysis

25. **PROCESSING AND RECYCLING OF ALUMINUM WASTES**
$111,000
DOE Contact: Simon Friedrich (202) 586-6759

This project at Michigan Technological University focuses on the development of a technology to divert the salt cake into valuable feedstock materials for the manufacturing of concrete products such as lightweight masonry, foamed concrete, and mine backfill grouts. By using the unique properties inherent in the aluminum salt cake, this by-product can function as a foaming (air entraining) agent, and fine aggregate for use in concrete. The technology is expected to benefit the aluminum, concrete, mining and construction industries. The aluminum industry will be able to increase its recovery of aluminum metal while reducing energy consumption. Technology development objectives include:

- Process by-product waste streams from several aluminum smelters and optimizes the processing required to convert wastes into products suitable for use as concrete additives.
- Develop and demonstrate the processing required to effectively utilized the processed by-products developed for the production of mine backfill grouts.
- Develop and demonstrate the processing required for lightweight aggregate/masonry block production utilizing the processed by-products developed.
- Document the environmental acceptability of the smelting by-products used as concrete additives and assess the environmental acceptability of the low-density concrete products made using these additives.

Keywords: Salt Cake, Recycling, Feedstock, Waste Streams, Concrete Additives

26. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$720,000

DOE Contact: Simon Friedrich (202) 586-6759

Reynolds Metals Company, Kaiser Mead, and Advanced Refractory Technologies (ART) will collaborate to develop and evaluate ceramic-based materials, technology, and the necessary engineering packages to retrofit existing reduction cells as a means to improve the performance of the Hall Héroult cell. ART will produce TiB_2-based tiles or coatings that will be used as the “drained” lining in two 70 kA prebake cells. The durability of the candidate materials and the performance of the drained cathode design will be evaluated during a one-month test using 12 kA pilot reduction cells. This four-year project, initiated in September 1997, will include the following activities:

- Development and evaluation of candidate TiB_2 carbon materials (tiles and coating)
- Development and evaluation of proprietary carbon materials
- Development of the drained cathode design
- Evaluation of the best candidate materials and the drained cathode design in the 12 kA pilot cell
- Design and construction of a 70 kA prebake cell retrofitted with a drained cathode using TiB_2-based and or the proprietary materials
- Startup and operation of two 70 kA prebake cells retrofitted with a drained cathode and TiB_2 and or the proprietary materials

Keywords: Cathode, Aluminum Production, Titanium Diboride

27. **SPRAY ROLLING ALUMINUM STRIP**
$269,000
DOE Contact: Ramesh Jain (202) 586-2381
INEEL Contact: Kevin McHugh (208) 525-5713

Alcoa Incorporated, Century Aluminum, Colorado School of Mines, Idaho National Engineering and Environmental Laboratory, Inductotherm, Metals Technology, and University of California are project partners for the development of a new process that combines benefits of twin-roll casting and spray forming. Aluminum’s competitive edge arises from the ease with which shapes can be extruded. Nearly all aluminum strip is manufactured commercially by conventional ingot metallurgical (I/M) processing, also known as continuous casting. This method accounts for about 70 percent of domestic production. However, it is energy and capital equipment intensive. Spray forming is a competitive low-cost alternative to ingot metallurgy for manufacturing ferrous and non-ferrous alloy shapes. It produces materials with a reduced number of processing steps, while maintaining materials properties, with the possibility of near-net-shape manufacturing. However, there are several hurdles to large-scale commercial adoption of spray forming: 1) ensuring strip is consistently flat, 2) eliminating porosity, particularly at the deposit/substrate interface, and 3) improving material yield. Researchers are investigating a spray rolling approach to overcome these hurdles. It should represent a processing improvement over conventional spray forming for strip production. Spray rolling is an innovative manufacturing technique to produce aluminum net-shape products. It requires less energy and generates less scrap than conventional processes and, consequently, enables the development of materials with lower environmental impacts in both processing and final products. It combines benefits of twin-roll casting and conventional spray forming.

Keywords: Aluminum, Spray Forming, Aluminum Strip and Sheet

28. **MODELING OPTIMIZATION OF DIRECT CHILL CASTING**
$644,000
DOE Contact: Simon Friedrich (202) 586-6759

The direct chill (DC) casting process is used for 68 percent of the aluminum ingots produced in the U.S. Ingot scrap from stress cracks and butt deformation account for a 5 percent loss in production. The basic process of DC casting is straightforward. However, the interaction of process variables is too complex to analyze by intuition or practical experience. The industry is moving toward larger ingot cross-sections, higher casting speeds, and an increasing array of mold technologies to increase overall productivity. Control of scrap levels is important in terms of both energy usage and cost savings. Predictive modeling and increasing the general knowledge of the interaction effects should lower production losses to 2 percent. This reduction in scrap could result nationally in an estimated annual energy savings of over six trillion Btu and cost savings of over $550 million by 2020. The DC casting model project focuses on developing a detailed model of heat conditions, microstructure evolution, solidification, strain/stress development, and crack formation during DC casting of aluminum. This model will provide insights into the mechanisms of crack formation, butt deformation, and aid in optimizing DC process parameters and ingot geometry. Project partners include Secat Inc., assisted by Alcan Aluminum Corp., ARCO Aluminum Inc., Logan Aluminum Inc., McCook Metals, LCC, Wagstaff Inc., Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Aluminum Ingot, Direct Chill Casting, Aluminum Scrap

FOREST AND PAPER PRODUCTS VISION TEAM

The DOE works in partnership with the forest products industry through the American Forest and Paper Association to develop cleaner, more energy-efficient technologies and processes to boost the productivity and profitability of the forest and paper products industry. The DOE Forest and Paper Products Team contact is Valri Robinson (202) 586-0937.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

29. **CORROSION IN KRAFT DIGESTERS: CHARACTERIZATION OF DEGRADATION AND EVALUATION OF CORROSION CONTROL METHODS**
$750,000
DOE Contact: David Boron (202) 586-0080
ORNL Contact: James Keiser (865) 574-4453

This project will correlate chemical pulping digester conditions with material performance. Digester conditions will be evaluated using a computational fluid dynamics model of flow within a digester. This flow model will be supplemented with a model for the chemical reactions occurring in the digester. *In situ* and laboratory corrosion studies will be used to provide information about the corrosion behavior of conventional materials. An assessment of corrosion control methods and alternative materials will be performed. This is a 5-year project with an expected completion date of 9/30/03.

Keywords: Digester, Corrosion, Pulp and Paper

30. **SELECTION AND DEVELOPMENT OF REFRACTORY STRUCTURAL MATERIALS FOR BLACK LIQUOR GASIFICATION**
$300,000
DOE Contact: David Boron (202) 586-0080
ORNL Contact: James Keiser (865) 574-4453

This project will identify refractory materials that have acceptable life to allow gasifiers to efficiently and economically operate using black liquor or biomass as feedstocks. Working with industrial partners, the investigators will identify and address the most serious material problems associated with the top three emerging biomass and black liquor gasification technologies. Studies will be performed to identify or develop more suitable materials for these applications. This is a 4-year project with an expected completion date of 9/30/03.

Keywords: Gasification, Black Liquor, Refractory, Pulp and Paper

METAL CASTING VISION TEAM - The DOE Metalcasting program manager is Harvey Wong (202) 586-9235

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

31. **CREEP RESISTANT ZINC ALLOY DEVELOPMENT**
$132,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
International Lead Zinc Research Organization Contact: Frank Goodwin (919) -361-4647

The objective of this project is to develop a hot chamber castable zinc die casting alloys that is capable of satisfactory service at 1400°C and preferably at moderately elevated temperatures 160°C. The target strength at this temperature is 4,500 psi during an exposure time of 1,000 hours. The project will be accomplished by enhancing a previously existing computer model relating zinc alloy composition to creep strength, followed by preparation of selected zinc die casting metal alloys and pressure die casting of these alloys. Mechanical testing will be carried out. An optimization task will then be conducted and these alloys will then be characterized in a manner similar to the first group of alloys. This task will be followed by technology transfer to die casters and their customers, concerning properties and processing of these enhanced alloys.

Keywords: Zinc Alloys, Zinc Die Casting, Creep Resistant

32. **DEVELOPMENT OF SURFACE ENGINEERED COATINGS FOR DIE CASTING DIES**
$149,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Colorado School of Mines Contact: John Moore (303) 273-3770

The objective of this research project is to develop a coating system that minimizes premature die failure (heat checking, erosive, and corrosive heat), and extend die life. No single (monolithic) coating is likely to provide the optimum system for any specific die casting application that will require its own specially designed "coating system". An optimized coating system will require a multi-layer "architecture" within which each layer provides a specific function, e.g. adhesion to the substrate, accommodation of thermal and residual stresses, wear and corrosion/oxidation resistance and non-wettability with the molten metal. The initial research project will concentrate on developing a coating system for dies used in die casting aluminum alloys. The measured outcomes from this research program will quantify comparisons of current aluminum die casting practice with the measured results using the newly developed coating systems. A comparison of cost/performance will also be determined for the new coating systems using current cost data as the base line.

Keywords: Surface Coatings, Multi-Layered-Surface Coatings, Die Casting, Die Casting Dies

33. **INTEGRATION OF RSP TOOLING WITH RAPID PROTOTYPING FOR DIE-CASTING APPLICATION**
$92,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Colorado State University Contact:
James Folkstead (970) 491-7823

The objective of the project is to utilize a rapid-tooling technology that will reduce the lead time for prototype and production die-casting tooling starting from a CAD drawing. Currently, there is no commercially available rapid tooling technology that satisfies the needs of the die casting industry. Compared to rapid tooling technologies for plastic injection molding and other plastic forming methods, rapid tooling options for die casting are very limited.

Keywords: Metalcasting, Die Casting, Rapid Tooling

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

34. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
$332,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates (205) 975-8011

This project is an extension to the Clean Cast Steel project, with the goal to improve casting product quality by removing or minimizing oxide defects and allowing the production of higher integrity castings for high speed machining lines. There are two objectives in this project, with the first one to identify the metallurgical factors influencing machinability of steel to gain an engineering understanding of the mechanism. A series of tests of commercial parts from participating foundries will be performed to evaluate the machinability. Factors to be examined include furnace practice, deoxidation practice, calcium wire injection, and heat treatment. The second objective is to provide the steel foundry industry with the technical resources needed to implement clean cast steel technology.

Keywords: Metalcasting, Steel Casting, Machinability

35. **PREVENTION OF POROSITY IN IRON CASTINGS**
$45,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Climax Research Services Contact: James Lakin
(248) 960-4900, Ext. 210

The objective of this research project is to understand porosity formation in castings, to generate fundamental materials data relevant to porosity formation, and to develop a method by which metalcasters can predict the porosity problem and make the necessary adjustments to prevent it. This will be accomplished by developing an understanding of the mechanisms for pore formation in castings, and developing a model for the use of the metal casting industry. This model will take into account all the factors affecting porosity formation. This model will help iron foundries to predict the conditions that are conducive to porosity formation in castings, and to take measures to prevent porosity.

Keywords: Metalcasting, Cast Iron, Porosity

36. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$325,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates (205) 975-8011

The objective of this project is to advance the state of the art in Lost Foam Casting technology. It is being carried out at the Lost Foam Technology Center at the University of Alabama at Birmingham. The project provides a means for designers, manufacturers, and purchasers/users of cast metal parts to harvest the benefits of the lost foam process, and furnishes project participants the best available technology. The current research focus is on the general technical areas of casting dimensional precision and freedom from casting defects in aluminum and cast iron. Tasks include foam pyrolysis defects, coating technology, pattern materials and production, computational modeling, casting distortion, and technology transfer.

Keywords: Metalcasting, Lost Foam Casting

37. **METALLIC REINFORCEMENT OF DIRECT SQUEEZE DIE CAST ALUMINUM ALLOYS**
$100,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Case Western Reserve University Contact:
Jack Wallace (216) 368-4222

The objectives of the project are to: 1) develop commercially feasible methods of reinforcing aluminum die castings with strong, tough metal inserts, 2) select aluminum alloys for the matrix and customize the type of insert depending on the application, 3) optimize interfacial coatings to provide a strong metallurgical bond between the insert and aluminum alloy, and 4) evaluate the mechanical properties of the reinforced castings.

Research includes fracture toughness and ballistic evaluation to be conducted at LANL.

Keywords: Metalcasting, Squeeze Casting, Aluminum, Reinforcement

38. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$70,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Tennessee Contact: Carl Lundin (423) 974-5310

Duplex stainless steel castings are receiving greater attention since the use of wrought duplex components is on the increase. The duplex stainless steels are now often considered for severe service because of their unique properties with regard to corrosion resistance (especially pitting resistance), strength and toughness. Unfortunately, a standardized method does not currently exist for calibrating instruments for the direct assessment or measurement of the ferrite-austenite phase relationships. The objective of this project is to develop calibration standards that will be applicable to duplex stainless steel castings and which will cover the full spectrum of the traditional duplexes and the newly-introduced super duplex , which contains special alloy additions for enhanced properties.

Keywords: Metalcasting, Calibration, Duplex Stainless Steel

39. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$215,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact: Charles Bates (205) 975-8011

The primary focus of this project is to determine how the machinability of gray and ductile iron castings can be improved to support the development of thin walled gray and ductile iron castings for use in the ground transportation industry. Excessive microcarbides have been found in prior research to be a dominant factor degrading machinability of iron castings. One of the major emphases is to determine how the occurrence of microcarbides can be controlled by normal foundry processing changes.

Keywords: Metalcasting, Gray Iron, Cast Iron, Inclusions, Machinability

40. **IMPROVEMENTS IN SAND MOLD/CORE TECHNOLOGY: EFFECTS ON CASTING FINISH**
$176,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Ohio State University Contact: John Lannutti (614) 292-4903

The overall objective of the project is to develop a fundamental understanding of how sand structure controls the final casting finish of metal castings made using sand molds and cores. In this project, Ohio State University will undertake a study of the effects of mold/core uniformity by combining an advanced non-destructive x-ray analysis and an optical profiler. The project will generate a fundamental understanding of how metal surfaces form in contact with sand molds/cores. The effort will focus on chemically bonded sands.

Keywords: Metalcasting, Sand Mold, Casting Finish

41. **HEAT CHECKING AND WASHOUT OF SUPERALLOYS FOR DIE INSERTS**
$100,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Case Western Reserve University Contact: Jack Wallace (216) 368-4222

The project has three main objectives: 1) develop and evaluate nickle and cobalt-base superalloys for use as inserts in die casting of aluminum alloys, 2) design and run a full size "erosion test" for evaluating washout in die insert materials, and 3) study the mechanisms of thermal fatigue crack nucleation and propagation in superalloys and compare these to thermal fatigue cracking of steels.

Keywords: Metalcasting, Die Casting, Heat Checking, Inserts

OFFICE OF CROSSCUT TECHNOLOGIES

INDUSTRIAL MATERIALS FOR THE FUTURE (IMF) PROGRAM

New or improved materials can save significant energy and improve productivity by enabling systems to operate at higher temperatures, last longer, and reduce capital costs. The Industrial Materials for the Future (IMF) program is a crosscutting program with emphasis on meeting the industrial needs of the Industries of the Future effort and of crosscutting industries including the carbon products, forging, heat treating, process heating, and welding industries. Efforts in FY 2001 were focused on development of 1) a new IMF program plan, 2) issuing three calls for proposals related to the industry, academia, and national laboratory sectors, and 3) continuation and completion of projects funded through the Advanced Industrial Materials (AIM) and the Continuous Fiber Ceramic Composites (CFCC) programs. The DOE program managers are Charles A. Sorrell (202) 586-1514 and Mike Soboroff (202) 586-4936.

MATERIALS PREPARATION, SYNTHESIS,

DEPOSITION, GROWTH OR FORMING

42. **ADVANCED MATERIALS/PROCESSES**
$1,090,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contact: P. Angelini (423) 574-4459

The goals of this project are to develop new and improved materials and materials processing methods. Metallic, intermetallic alloys, refractories and ceramics possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 2001, R&D also utilized the new 300,000 W high intensity infrared heating and processing system. Research conducted related to surface modification of ceramics, refractory and alloy systems; materials properties, thermodynamics, and high temperature filtration materials.

Keywords: Intermetallic, Alloys, Metalcasting, Glass, Alloys, Welding, Corrosion Resistance, Infra Red Heating, Coatings, Refractories, WC, Thermodynamics, Materials Properties, Thermal Spray

43. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
$300,000
DOE Contact: Charles A. Sorrell (202) 586-1514
Sandia National Laboratories Contact:
R. E. Loehman (505) 844-2222
(includes effort on coating technology at Stanford Research Institute)

Ceramic-metal composites have advantages as engineering materials because of their high stiffness-to-weight ratios, good fracture toughness, and because their electrical and thermal properties can be varied through control of their composition and microstructure. Reactive metal infiltration is a promising new route to synthesize and process a wide range of ceramic and metal-matrix composites to near-net-shape with control of both composition and microstructure. In FY2001, development of the technique was continued and various materials were evaluated.

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics, Composites, Inorganic Coatings, Corrosion

44. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
$150,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory Contact:
S. Gottesfeld (505) 667-0853

In FY 2001, the use of conducting polymers for electrochemical reactors (ECRs) based on polymeric electrolytes was addressed. The objective of this effort is to develop and test electrochemical reactors for the chlor-alkali industry, based on polymer membrane/ electrode assemblies and on oxygen or air electrodes. In FY 2001, development of the oxygen polarized chlor-alkali cells was continued.

Keywords: Electrically Conducting Polymers, Gas Separation, Electrochemical Reactors, Cathodes

45. **DEVELOPMENT OF ADVANCED METALLIC/INTERMETALLIC ALLOYS**
$670,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contact: P. J. Maziasz (423) 574-5082,
M. L. Santella (423) 574-4805, V. K. Sikka (423) 574-5112 and C. T. Liu (423) 574-4459

The objectives of this project are to develop advanced intermetallic alloys including FeAl and Ni_3Si. The FeAl effort is focused on alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and the development of weldable FeAl alloys for use in weld-overlay cladding applications. The Ni_3Si effort is focusing on alloy composition, and welding. Developments made in FY 2001 included 1) improvement of the ductility and joining of nickel silicide, 2) development of autogenous and dissimilar metal welding of iron aluminide, and 3) corrosion studies in carburizing environments.

Keywords: Iron Aluminides, Nickel Aluminides, Coatings, Claddings, Thermophysical Properties, Casting, Thermomechanical Properties, Chemical Industry, Steel Industry, Welding, Alloys

46. **HIGH TEMPERATURE FACILITATED MEMBRANES**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory: D. J. Devlin (505) 667-9914

The project focuses on the development of membranes and a test system for their evaluation. The purpose of the project is to develop and evaluate a new high-temperature membrane for the separation of carbon dioxide from hydrogen. The approach involves the use of molten carbonate type materials with reversibility, measurement of transport properites through membranes, and the evaluation of decomposition to oxide on the downstream side. In FY2001, progress was made in fabricating membranes of lithium carbonate on metallic substrates.

Keywords: Membranes, Liquid Vapor Separations, Oxygen, Carbon Dioxide, Natural Gas

47. **INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS**
$680,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contacts: M. L. Santella (423) 574-4805 and V. K. Sikka (423) 574-5112
University of Tennessee, G. M. Pharr (865) 974-8202

The objective of this project is to develop and apply the excellent oxidation and carburization resistance and higher strength of intermetallic alloys including nickel aluminides to Industries of the Future related manufacturing applications. Progress in bringing technologies to development and commercialization in FY 2000 included: 1) processing of radiant tubes and rolls for testing and evaluation, 2) the evaluation of long term stability tests of nickel aluminide, and 3) joining technology for the iron aluminide system.

Keywords: Nickel Aluminides, Processing, Steel, Metalcasting, Heat Treating, Welding, Chemical, Properties

48. **PLASMA PROCESSING-ADVANCED MATERIALS FOR CORROSION AND EROSION RESISTANCE**
$300,000
DOE Contact: Charles A. Sorrell (202) 586-1514
Los Alamos National Laboratory: M. Trkula (505) 667-0591

The project focuses on developing coating technologies to obtain erosion, and corrosion resistant, thermodynamically stable, and adherent coatings on die materials used to cast aluminum and other metals. Low temperature organo-metallic chemical vapor deposition combined with immersion ion processing are being developed as the coating technology. In FY 2001, various coatings were produced on substrates and evaluated.

Keywords: Plasma, Processing, Corrosion, Erosion, Coatings, Materials

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

49. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) - SUPPORTING TECHNOLOGIES**
$1,150,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

This project provides basic or generic support to the industry teams conducting the CFCC process research and development. Tasks include: composite design, materials characterization, test methods development, database generation, codes and standards, and life prediction.

Keywords: Ceramic Composites, Materials Characterization, Test Methods, Life Prediction

50. **MATERIALS DEVELOPMENT FOR THE FOREST PRODUCTS INDUSTRY**
$980,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contact: Peter Angelini (423) 574-4565

The purpose of this project is to determine the cause of failure of composite tubes used in Kraft Black Liquor recovery boilers during pulp and paper making, and to develop new materials to eliminate failures. The project consists of three efforts: 1) to obtain operating data and failure analyses, 2) determination of residual stresses in new and used composite tubes and microstructural characteristics of tubes, and 3) development of new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. In FY 2001, the main effort was related to the materials behavior of wall tubes specifically near air ports of kraft recovery boilers. Various companies continued installation of retrofitted parts of floors with the new materials. Temperature measurements of tubes at air ports were continued and results highlighted the influence and significance of thermal cycling on the corrosion/cracking behavior of tubes at those locations. Participants include Oak Ridge National Laboratory (ORNL), Institute of Paper Science and Technology (IPST), the Pulp and Paper Research Institute of Canada (PAPRICAN), 18 pulp and paper companies, and 6 boiler and materials suppliers.

Keywords: Corrosion, Recovery Boilers, Composite Tubes, Pulp and Paper, Alloys, Stresses, Neutron Residual Stress, Measurements, Modeling, Mechanical Properties

51. **METALS PROCESSING LABORATORY USERS (MPLUS) FACILITY**
$550,000
DOE Contact: Charles A. Sorrell (202) 586-1514
Oak Ridge National Laboratory Contact: P. Angelini (865) 574-4565

The Metals Processing Laboratory User (MPLUS) Facility is an officially designated DOE User Facility. Its primary focus is related to the Office of Industrial Technologies (OIT) efforts including the "Industries of the Future," national, and cross cutting programs. The purpose of MPLUS is to assist U.S. industry and academia in improving energy efficiency and enhancing U.S. competitiveness. MPLUS includes the following user centers: Metals Processing, Metals Joining, Metals Characterization, and Metals Process Modeling. As of the end of FY 2001, 0ver 160 proposals were received with over 60 MPLUS projects having been completed. Projects crosscut all of the industries in the Industries of the Future effort and other supporting industries including forging, heat treating, welding.

Keywords: Industry, User Center, Metals, Materials, Processing, Joining, Properties, Characterization, Modeling, Process

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

52. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) - INDUSTRIAL TECHNOLOGIES**
$1,500,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

The Continuous Fiber Ceramic Composites (CFCC) activity operates as a collaborative effort between industry, national laboratories, universities, and the government to develop advanced ceramic composite materials to a point at which industry will assume full risk of further development. Various industry projects were completed. National laboratories, along with universities, continued the development of supporting technologies (e.g., materials design, processing methods, and sensing technologies) and conducting performance based evaluations. The DOE program manager is Mike Soboroff (202) 586-4936.

Keywords: Continuous Fiber Ceramic Composites, Materials Processing

53. **SELECTIVE INORGANIC THIN FILMS**
$250,000
DOE Contact: Mike Soboroff (202) 586-4936
Sandia National Laboratories contact:
T. M. Nenoff (505) 844-0340

The purpose of this research is to develop a new class of inorganic zeolite based membranes for light gas separation and use this technology to improve on separation efficiencies currently available with polymer membranes, particularly for light alkanes. The approach is to nucleate and crystallize zeolithic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. In FY2001, the R&D continued with advancements made in the fabricability of membrane systems.

Keywords: Coatings, Sol-Gel Processing, Membranes, Separations, Zeolite

INDUSTRIES OF THE FUTURE MATERIALS ISSUES

54. **IMF CALL FOR PROPOSALS FOR 2001**
$4,500,000
DOE Contact: Charles Sorrell (202) 586-1514 and Mike Soboroff (202) 586-4936

The IMF program issued a call for proposals in FY 2001 addressing materials issues related to the Industries of the Future activities. The topics included corrosion resistant materials, high temperature materials, coatings and surface treatments, materials data bases and other topics. The call requested proposals from the industrial, academia, and national laboratory sectors and initial selections were made.

Keywords: Materials, Alloys, Refractories, Ceramics, Coatings, Surface Modification, Data Bases, Properties, Materials Modeling, Corrosion, Membranes, Nanomaterials, High Temperature Materials

FINANCIAL ASSISTANCE PROGRAM

The goal of the Financial Assistance Program of OIT is to support technologies within the areas of industry, power, transportation, or buildings that have a significant energy savings impact and future commercial market potential. OIT is particularly interested in supporting technology development and deployment in OIT's "Industries of the Future," nine of the most energy-intensive U.S. industries-agriculture, aluminum, chemicals, forest products, glass, metalcasting, mining, petroleum, and steel industries. Financial assistance through a competitive solicitation is offered to: 1) speed the development of new energy efficient inventions, and 2) leverage industry and other resources to demonstrate, and promote the benefits of energy savings, pollution prevention and cost savings possible through the adoption of clean, energy-efficient industrial technologies. OIT provides grants and assistance to independent inventors and small businesses with promising new ideas through its inventions and innovation (I&I) Program. OIT also provides grants to help fund technology demonstrations through its National Industrial Competitiveness through Energy, Environment and Economics ($NICE^3$) Program.

INVENTIONS AND INNOVATION
DOE Contact Lisa Barnett (202) 586-2212

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

55. **LASER SENSOR FOR OPTIMIZATION OF COMPRESSOR STATIONS AND REFINERY OPERATIONS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
LaSen, Inc. Contact: Allen R. Geiger
(505) 522-5110

LaSen, Inc. will develop a process to rapidly monitor and inspect leaks associated with valves and flanges within natural gas and liquid pipeline compressor stations. If a proposed detection system is installed in a petroleum refinery, product savings and associated embodied energy savings could reach $1-2 million/year.

Keywords: Laser, Leak Detection, Natural Gas, Pipeline

56. **TITANIUM MATRIX COMPOSITE TOOLING MATERIAL FOR ENHANCED MANUFACTURE OF ALUMINUM DIE CASTINGS**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
Dynamet Technology, Inc. Contact:
Susan Abkowitz (781) 272-5967

The grant will be used to produce a metal matrix composite material composed of Ti-6Al-4V and 10 wt% titanium carbide particulate. The titanium metal matrix composite offers both dramatically improved (400 percent) durability and reduced thermal conductivity (50 percent compared to steel) which will provide energy savings by reducing preheating energy consumption by 4-8 percent.

Keywords: Metal Matrix Composite, Titanium, Aluminum, Die Casting

57. **AN INSOLUBLE TITANIUM-LEAD ANODE FOR SULFATE ELECTROLYTES**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
Electrodes International, Inc. Contact:
Alla Ferdman (847) 465-0785

The grant will be used to develop insoluble anodes for electrowinning of metals such as copper, zinc, nickel, cobalt, etc. and for electrolytic manganese dioxide production. The proposed anodes significantly reduce contamination of the products with lead and can be used at lower voltage and increased current density, resulting in higher productivity and energy savings up to 25 percent.

Keywords: Electrowinning, Anodes

58. **DEVELOPMENT OF AN INNOVATIVE ENERGY EFFICIENT HIGH TEMPERATURE NATURAL GAS FIRED FURNACE**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Procedyne Corp. Contact: Vijay Shroff
(732) 249-8347

The grant will be used to improve the efficiency of gas-fired furnaces used for heat-treating, metal recovery, and inorganic chemical production. Compared to current gas-fired heating mantles, the proposed furnace can save up to 70 percent of natural gas fuel and achieve a higher combustion efficiency for a given combustion gas discharge temperature.

Keywords: Heat Treating, Gas-fired Furnaces

59. **A NEW HIGH TEMPERATURE COATING FOR GAS TURBINES**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
Turbine Coating, Inc. Contact: Maggie Zheng
(518) 348-0551

The grant will be used to develop a new coating with cracking resistance and enhanced oxidation protection for hot section components of gas turbines. Energy savings will be derived from reducing one of the two traditional coating steps and extending component life.

Keywords: Coatings, Gas Turbines

60. **TOUGH-COATED HARD POWDERS (TCHPs): A NEW PARADIGM IN MINING AND MACHINING TOOL MATERIALS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
EnDurAloy Corp. Contact: Rick Toth
(912) 598-1210

The grant will be used to demonstrate a new process to sinter tungsten carbide particles resulting in increased hardness, strength, and abrasion resistance with the potential to extend tool life 10-25 times.

Keywords: Tungsten Carbide, Wear Resistant Tools

[1]Prior year funding

61. **A NEW ENERGY SAVING METHOD OF MANUFACTURING CERAMIC PRODUCTS FROM WASTE GLASS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Haun Labs Contact: Michael Haun (707) 538-0584

The grant will be used to develop a new method to lower energy costs of manufacturing ceramic products. The process calls for the substitution of traditional raw materials with waste glass. Melting temperatures and associated energy consumption will decrease by 35-50 percent by sintering glass powder instead of using traditional ceramic materials.

Keywords: Cullet, Ceramic, Sintering Glass Powder

62. **DISTILLATION COLUMN FLOODING PREDICTOR**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Inventor Contact: George Dzyacky (219) 365-8336

The grant will be used to develop a pattern recognition system that identifies patterns of instability in a petroleum refinery distillation tower prior to flooding. The technology is credited with de-bottlenecking refinery processes and increasing gasoline production by 5-7 percent.

Keywords: Distillation Column Flooding, Petroleum Refinery

63. **ENERGY SAVING LIGHTWEIGHT REFRACTORY**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Silicon Carbide Products, Inc. Contact:
David Witmer (607) 562-7585

The grant will be used to develop a new manufacturing technique to produce a unique silicon carbide based material that has high strength, increased high temperature qualities, and will cost less to manufacture. In addition, the new material has shown great promise in molten aluminum applications.

Keywords: Refractory, Silicon Carbide

64. **HIGH INTENSITY SILICON VERTICAL MULTI-JUNCTION SOLAR CELLS**
$0[1]
DOE Contact: Lizanna Pierce (303) 275-4727
PhotoVolt, Inc. Contact: Bernard Sater
(440) 234-4081

The grant will be used to develop a low-cost, high-volume fabrication process for high intensity vertical multi-junction (VMJ) solar cells and demonstrate performance viability in solar concentrators. The unique features of the VMJ cell make it capable of more efficient operation at higher intensities than other silicon concentrator solar cell designs.

Keywords: Solar Cells, Solar Concentrators, Photovoltaic

65. **FABRICATION AND TESTING OF A PROTOTYPE CERAMIC FURNACE COIL**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
FM Technologies, Inc. Contact: Ralph Bruce
(703) 425-5111

The grant will be used to demonstrate a process for joining pairs of ceramic tubes to fabricate furnace coils for ethylene production plants. Ethylene has the greatest annual production of any organic chemical and is the number one consumer of energy in the petrochemical industry. Replacement of metal alloy coils with ceramic coils could increase ethylene production by up to 10 percent leading to substantial energy savings and increased productivity.

Keywords: Ceramic Tubes, Furnace Coils, Ethylene Production

66. **GERMANIUM COMPOUNDS AS HIGHLY SELECTIVE FLUORINATION CATALYSTS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Starmet Corporation Contact:
Matthew Stephens (978) 369-5410

The grant will be used to demonstrate the concept for a new, highly selective catalyst for the fluorination of hydrocarbons. This catalyst will meet the needs of the fluorocarbon industry for process simplification, for reduction in capital costs, and for the elimination of energy intensive processing steps and separation processes.

Keywords: Germanium Compounds, Hydrocarbon Fluorination, Catalyst

[1]Prior year funding

67. **DEVELOPMENT OF PHOSPHORS FOR USE IN HIGH-EFFICIENCY LIGHTING AND DISPLAYS**
$0[1]
DOE Contact: Andy Trenka (303) 275-4745
Brilliant Technologies, Inc. Contact:
Douglas Kezler (541) 737-6736

The grant will be used to develop new phosphors for use in high-efficiency, LED-activated lamps and displays, providing improved color rendering and significant energy savings. The phosphors will provide for the first time a means to produce true tri-chromatic white light under LED excitation.

Keywords: Phosphors, LED-Activated Lamps, LED

68. **NOVEL CERAMIC COMPOSITION FOR HALL-HEROULT CELL ANODE APPLICATION**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Advanced Refractory Technologies, Inc. Contact:
Thomas Mroz (716) 875-4091

The grant will be used to develop a replacement for traditional carbon anodes with non-consumable material that will reduce primary aluminum production costs, reduce energy consumption by up to 20 percent, and minimize environmental impact. The proposed project will evaluate ceramic material in anode-simulation conditions for corrosion and oxidation resistance, electrical properties, and cost efficiency compared to carbon anodes.

Keywords: Hall-Heroult, Anode, Aluminum Production

69. **FUNCTIONALLY GRADED MATERIALS FOR IMPROVED HIGH TEMPERATURE PERFORMANCE OF Nd-Fe-B-BASED PERMANENT MAGNETS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Iowa State University Contact: Alan Russel
(515) 294-3204

The grant will be used to develop a processing method to produce a novel microstructure in Nd-Fe-B-type magnets by use of pulsed laser deposition. This method is projected to increase the useful operating temperature by 115˚C and will substantially expand potential applications allowing Nd-Fe-B-type magnets to replace weaker magnets required for elevated temperature use. These magnets could reduce the weight of automobile starter motors by 14 lbs. resulting in improved overall gas mileage.

Keywords: Nd-Fe-B Based Magnets, Permanent Magnets, Pulse Laser Deposition

70. **IMPROVED ALKYLATION CONTACTOR**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
VHP, Inc. Contact: Jim Vemich (801) 397-1983

The grant will be used to develop a new type of contactor that will significantly increase the surface area between the hydrocarbon and acid catalyst phases while greatly reducing the mass transfer resistances by improved convection. Benefits from the new process include reducing acid consumption by at least 50 percent, improving the octane number of gasoline, eliminating the energy currently used to chill the reactants and acid below ambient temperature, and increasing the yield of high-octane gasoline.

Keywords: Alkylation, Petroleum Refining, Acid Catalyst

71. **LOW COST SYNTHESIS AND CONSOLIDATION OF TiC**
$0[1]
DOE Contact: David Blanchfield (303) 275?4797
The University of Idaho, Institute for Materials and Advanced Processes Contact: F.H. Froes, (208) 885-7989

The grant will be used to demonstrate a cost-affordable process for the synthesis of ultrafine titanium carbide (TiC) powder from low cost precursors by an ambient temperature mechanochemical process to form fine grained metal matrix composites. The proposed ambient temperature process will use less energy compared to other carbide manufacturing processes and the quality of the synthesized TiC is superior in purity and particle size to conventional products.

Keywords: Titanium Carbide Powder, Metal Matrix Composites

72. **DEVELOPMENT OF ALUMINUM IRON ALLOYS FOR MAGNETIC APPLICATIONS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Magna-Tech P/M Labs Contact: Kenneth Moyer
(856) 786-9061

The grant will be used to develop a powder metallurgy process to admix aluminum powder with iron powder to form iron alloy magnets. Upon sintering, a liquid phase is formed with superior magnetic properties to wrought alloys. When utilized in motor applications, the weight of small motors used in today's automobile may be reduced

[1]Prior year funding

by 15 percent and a 15-25 percent increase in motor efficiency may be realized.

Keywords: Powder Metallurgy, Aluminum Iron Alloys, Magnets

73. **NOVEL FREQUENCY-SELECTIVE SOLAR GLAZING SYSTEM**
$0[1]
DOE Contact: Andy Trenka (303) 275-4745
Orion Engineering, Inc. Contact: Thomas Regan (978) 589-9850

The grant will be used to develop a novel frequency-selective glass material for use in automobile, building, or solar-thermal collector application. This material is capable of transmitting selective frequencies of light with almost no reflection while efficiently transmitting visible light. The glazing could be used to minimize direct solar heating, resulting in reduced heating and cooling requirements for buildings and automobiles.

Keywords: Glazing, Windows, Frequency-Selective Glass

74. **A CERAMIC COMPOSITE FOR METAL CASTING**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
MER Corporation Contact: James Withers (520) 574-1980

The grant will be used to demonstrate nitride/nitride-carbide ceramic composite casting dies. Ceramic composite materials offer complete stability to molten metals and are resistant to erosion, oxidation, thermal fatigue, and cracking. The potential life span of ceramic composite dies could be ten times that of coated steel dies.

Keywords: Die Casting, Ceramic Composite, Metal Casting

75. **ELECTROCHEMICAL METHOD FOR EXTRACTION OF OXYGEN FROM AIR**
$0[1]
DOE Contact: Lizanna Pierce (303) 275-4727
James Mulvihill and Associates Contact: James Mulvihill (412) 221-2551

The grant will be used to develop a process to produce pure oxygen from air by combining the anode reaction of a water electrolysis cell and the cathode reaction of a fuel cell in a single unit. The combined cell requires less energy to produce pure oxygen compared with a standard water electrolysis cell.

Keywords: Water Electrolysis, Oxygen, Fuel Cell

76. **ENERGY SAVING METHOD FOR PRODUCING ETHYLENE GLYCOL AND PROPYLENE GLYCOL**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
Gallatin Research Contact: Warren Miller (541) 388-2198

The grant will be used to demonstrate a new process that could dramatically reduce the energy and water requirements in glycol production. Together, these two chemicals account for over 7 billion pounds of production consuming 33 trillion Btu and four billion gallons of water. The proposed process could reduce energy and water consumption by 20 percent.

Keywords: Glycol Production, Ethylene Glycol, Propylene Glycol

77. **IMPROVED REFRACTORIES USING ENGINEERED PARTICLES**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Powdermet, Inc. Contact: Andrew Sherman (818) 768-6420

The grant will be used to determine the technical feasibility of producing a higher thermal shock resistant carbon-alumina refractory by producing and testing engineered alumina particles. The novel material has the potential to increase refractory durability by three to five fold.

Keywords: Refractory, Carbon-Alumina, Thermal Shock

78. **ENABLING TOOL FOR INNOVATIVE GLASS APPLICATIONS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Michigan Technological University, Institute of Materials Processing Contact: J. M. Gillis (906) 487-1820

The grant will be used to develop an abrasive jet cutting system using glass as the abrasive media. Angular glass particles have been shown to be an acceptable alternative abrasive to garnet and at one-tenth the price of garnet, will allow for a wider array of glass products to be produced. Spent abrasive glass will be suitable for use as a plastic filler in a variety of polymers.

Keywords: Glass, Abrasive Jet Cutting System, Garnet

[1]Prior year funding

79. **DISTRIBUTED OPTICAL SENSORS FOR CONTINUOUS LIQUID LEVEL TANK GAUGING**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Project Contact: Joram Hopenfeld: (301) 340-1625

The grant will be used to develop a Noverflo multi-point tank gauging device that will be compact, sensitive, and manufactured inexpensively in large quantities. The sensor will not require special signal conditioning to interface with host computers and will save energy by reducing power requirements, optimizing fuel utilization, and reducing fuel leaks.

Keywords: Tank Gauging, Transportation, Tank Overfill Protection

80. **A LOW ENERGY ALTERNATIVE TO COMMERCIAL SILICA-BASED GLASS FIBERS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
MO-SCI Corporation Contact: Ted Day (573) 364-2338

The grant will be used to develop high strength, iron phosphate glass fibers for composites and other products in the transportation, aircraft, and chemical industries. Iron phosphate glasses have a chemical durability that exceeds many commercial silica-based glasses and can be melted 3 to 20 times faster at temperatures 400-600°C lower than commercial boro-alumino-silicate glass.

Keywords: Glass, Iron Phosphate Glass Fibers, Silica-Based Glass Fibers

81. **CROMER CYCLE AIR CONDITIONING**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
Solar Engineering Co. Contact: Charles Cromer (407) 638-1445

The grant will be used to develop the Cromer Cycle Air Conditioner that uses a desiccant to move moisture from the outlet duct to the inlet duct. This has the thermodymanic effect of reducing the overall energy consumption of the air conditioner and increasing the moisture removal capacity of the air conditioner coil resulting in a 16 percent reduction in energy consumption and a 47 percent improvement in EER.

Keywords: Air Conditioner, Desiccant, Moisture Removal

82. **A VIABLE INERT CATHODE FOR SMELTING PRIMARY ALUMINUM**
$40,000
DOE Contact: Keith Bennett (303) 275-4905
PRACSOL, LLC Contact: Robert Rapp (614) 292-6178

This grant is aimed at developing sufficient experimentation to prove the feasibility of a net shape method of manufacture and the effective properties of a porous TiB_2 body suitable as an inert cathode in the in the Hall-Heroult cell.

Keywords: Aluminum, Cathode, Inert Cathode, Titanium

83. **DEVELOPMENT OF INERT ANODE FOR THE PRIMARY ALUMINUM INDUSTRY**
$40,000
DOE Contact: Keith Bennett (303) 275-4905
Energy Research Company Contact: Robert De Saro (718) 442-2725

This grant will experimentally determine the amount and purity of the aluminum produced in a bench-scale Ionic Ceramic Oxygen Generator (ICOG) inert anode experiment and to determine anode degradation. The ICOG inert anode uses a crystal lattice to transport oxygen ions from the electrolytic solution where they are oxidized to diatomic oxygen gas. For this research project, the ICOG inert anode will replace the traditional consumable carbon anode in this project.

Keywords: Aluminum, Anode, Inert Anode, Anode Degradation

84. **CATALYTIC PROCESSORS FOR CO_2 REFORMING OF CH_4 AND GASEOUS HYDROCARBONS**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Contact: Zoe Ziaka-Vasileiadou - Individual Inventor (818) 893-4292

The objective of this grant is to develop effective CO_2-hydrocarbon reforming catalytic process with and without the use of steam in feed for reforming of acidic natural gas, landfill gas, sour gases, and flue gases with hydrocarbon molecules containing one to four carbon atoms. The products are hydrogen and carbon oxides to be subsequently used as a fuel in fuel cells, gas turbines-engines, or as synthesis gas (synthesis of methanol, ammonia, saturated alkanes). The work will also develop

[1]Prior year funding

effective process designs involving one or more vessels for reaction, separation, or combined reaction and separation within the same vessel.

Keywords: Hydrocarbon Reforming, Catalysis, CO_2, Reforming, Low Btu Fuel

85. **TESTING A HIGHLY EFFICIENT TECHNOLOGY FOR CONVERTING WOODY BIOMASS TO ELECTRICITY**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Gazogen, Inc. Contact: Syver Rogstad (802) 456-8163

This grant will construct a full scale, operational, prototype torrefier. The torrefier will be tested with our prototype gasifier. The prototype torrefier will enable efficiency improvement testing between torrefied and non-torrefied, dry and green, fuel.

Keywords: Biomass, Gasifier, Torrefier, Green Fuel

86. **AUTOMATIC EVALUATION OF WOOD PROPERTIES**
$39,896
DOE Contact: Doug Hooker (303) 275-4780
Quantum Magnetics Contact: Tracey Wrightson (858) 566-9200

The project objective is to determine quantitative, predictive formulas relating wood properties to the solid-state magnetic resonance measurement parameters through the species/class categorization. With the project funds, we will experimentally derive a wood species relationship in terms of magnetic resonance signal parameters, sufficient to allow pallet recyclers to sort wood parts knowing that the reassembled pallets will provide service at least equal to that of a new pallet from similar species material.

Keywords: Pallets, Wood Speciation, Magnetic Resonance, Wood Sorting

87. **IMPROVED PROCESS CONTROL OF WOOD WASTE FIRED BOILERS**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Process Control Solutions, Inc. Contact: Rick Meeker (850) 385-5100

The purpose of this grant is to fully characterize the wood-waste boiler control inter-relationships and constraints through data collection and analysis, design an improved control architecture, develop and test an appropriate model predictive control and optimization algorithm, and develop and test a procedure for reproducing the approach and deriving the benefits on all similar pulp and paper wood-waste boilers.

Keywords: Wood-Waste Boiler, Pulp and Paper Boilers, Boiler Architecture

88. **ENERGY-EFFICIENT PRODUCTION AND UTILIZATION OF LIGHT-WEIGHT STRUCTURAL PANELS**
$40,000
DOE Contact: Gibson Asuquo (303) 275-4910
Genesis Laboratories, Inc. Contact: Thomas Owens (630) 879-1112

The primary objective of this grant is to demonstrate the feasibility and energy savings of the MWAC method for consolidating and finishing structural cores used in the production of light-weight sandwich panels.

Keywords: Structural Panels, Building Panels, Sandwich Panels

89. **HIGH PURITY FUSED SILICA GLASSES**
$40,000
DOE Contact: Gibson Asuquo (303) 275-4910
Rensselaer Polytechnic Institute Contact: Patricia Gray (518) 273-6659

This grant will prepare high purity silica glasses and demonstrate their superior characteristics. High purity silica glasses with superior quality proposed in this work will be supplied to both electronics industry and to optical fiber manufacturers. At the present time, no one holds the technology rights on the proposed method of high purity silica glass production.

Keywords: Glass, Optical Fiber, High Purity Silica

90. **BATCH PREHEAT FOR GLASS AND RELATED FURNACE PROCESSING OPERATIONS**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Energy and Environmental Resources Contact: William Fleming (765) 647-0076

This grant will consist of preparing various salt eutectics in the lab: chlorides of aluminum, iron (III), sodium, calcium, and magnesium will be used in these formulations. The salts will be dissolved in various proportions, and then the water will be evaporated off. Melting points will then be determined in a muffle furnace. The samples which have melting points in the 200-300°F range will then be tested further: in these test, the eutectic salts will be subjected to high temperature exposure (up to 1800°F) in a small lab kiln. The samples will be evaluated thermal stability based on weight loss or evolution of gas/vapor, etc. The eutectic salts will be rated for thermal stability with the top 2 or 3 being tested for corrosivity. The salts will then be used on various metal alloys at up to 1800°F. Finally, corrosivity test will be conducted with metal alloys subjected to sodium sulfate at up to 1800°F.

Keywords: Glass, Glass Furnace, Eutectic Salts, Metal Alloys

91. **DEVELOPMENT OF ENVIRONMENTALLY BENIGN MINERAL FLOTATION COLLECTORS**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Versitech, Inc. Contact: Sharon Young
(520) 742-9457

The objective of this grant is to determine the precise factors that allow the non-sulfur containing triglycerides to collect sulfide minerals, particularly copper, as well or better than the conventional sulfur-containing collectors. The physical and chemical properties of the oils will be measured to try to obtain a correlation between one or more properties or compositions and mineral recoveries. To assist in this effort, artificial oils composed of one type of triglyceride will be tested in order to try to elucidate the best composition for a particular type of ore.

Keywords: Mining, Mineral Flotation, Sulfides, Copper

92. **A MICROBIAL GENOMICS APPROACH TO RESOURCE EXPLORATION AND CHARACTERIZATION**
$40,000
DOE Contact: Roxanne Danz (303) 275-4706
Taxon Biosciences, Inc. Contact: Matt Ashby
(415) 381-3554

The objective of this grant is to perform a feasibility study of Taxon's microbial survey technology and is comprised of the following objectives: 1) Conduct a survey of microbial diversity from 10 environmental samples; 2) Create a database of the microbial diversity profiles from these samples; 3) Perform correlation analyses between microbial markers and environmental parameters, and 4) Verify the identity of the microbial markers and their correlation with a given parameter.

Keywords: Microbes, Environmental Characterization, Soils

93. **NEW MEMBRANE PROCESS FOR IMPROVED ENERGY SAVING SEPARATIONS IN THE PETROLEUM INDUSTRY**
$40,000
DOE Contact: Doug Hooker (303) 275-4780
Contact: John Dorgan - Individual Inventor
(303) 277-9033

The objective this grant is to demonstrate a new membrane formation process employing a novel solvent and to demonstrate that the membranes produced possess superior properties when compared to existing materials.

Keywords: Petroleum Refining, Membranes, Separations

94. **COKE FORMATION PROCESS MODEL FOR PETROLEUM REFINING EFFICIENCY IMPROVEMENT**
$39,519
DOE Contact: Gibson Asuquo (303) 275-4910
Western Research Institute Contact:
John Schabron (307) 721-2445

The objective of this grant is to determine the Coking Indexes with a residuum material, which will be pyrolyzed, and to explore potentially simpler analytical measurements that may correlate with the indexes such that real-time feedback and refinery process control is attained.

Keywords: Petroleum Refining, Coking Indexes, Refinery Process Controls

95. **FLUTED SPIRAL MEMBRANE MODULE FOR REVERSE OSMOSIS OF LIQUIDS WITH DISSOLVED AND SUSPENDED SOLIDS**
$40,000
DOE Contact: Doug Hooker (303) 275-4780
Scinsep Systems Contact: Jatal Mannapperuma
(530) 758-3708

The objectives of this grant are to develop a methodology for the fabrication of the fluted spiral module, produce a prototype module and test its performance.

Keywords: Fluted Spiral Membranes, Reverse Osmosis, Separations

96. **ELECTROCHROMIC WINDOW FILM**
$40,000
DOE Contact: Andy Trenka (303) 275-4745
Chameleon Optics, Inc. Contact: Paul Martin
(215) 387-2717

This grant will demonstrate manufacturing feasibility of electrochromic window films and to produce samples for further evaluation.

Keywords: Electrochromic Windows, Buildings, Window Film

97. **PROCESS PARTICLE COUNTER (PPC) SENSOR/CONTROLLER FOR OPTIMIZING POWER RECOVERY EXPANDER AND GAS TURBINE PERFORMANCE FOR VARIOUS FUEL SOURCES**
$106,942
DOE Contact: Roxanne Danz (303) 275-4706
Process Matrix, LLC Contact: Donald Holve (925) 837-1330

This grant will perform short-term field measurements of current expanders/gas turbines to provide basic operating parameters (size and concentration). Measurements of particle loading will be obtained upstream and downstream of the turbines to determine actual turbine losses. If turbine losses are minimal, then it will be easier to perform monitoring measurements at the downstream location. This will determine the appropriate instrument interface with the turbine system. The new PPC design (optical configuration and interface) will then be implemented, followed by long-term testing at each application, expanders and gas turbines.

Keywords: Sensors and Controls, Gas Turbines, Particle Loading

98. **THERMOPHOTOVOLTAIC ELECTRIC POWER GENERATION USING EXHAUST HEAT IN THE GLASS, STEEL AND METAL-CASTING INDUSTRIES**
$199,806
DOE Contact: Gibson Asuquo (303) 275-4910
JX Crystals, Inc. Contact: Jason Keyes (425) 392-5237

The objective of this grant is to build a thermophotovoltaic (TPV) cylinder heated externally with a water-cooled TPV array inside. JX Crystals has developed TPV systems with burners that heat an emitter surrounded by TPV cells. For this project, the heat source is the exhaust stream from an industrial process, so the TPV geometry will be inverted and the circuits will be placed inside an emitter tube. JX Crystals plans to demonstrate the production of 1.5 W/cm^2 of electricity and a TPV efficiency of 20 percent. Additionally, Enron and other companies in the glass, steel and metalcasting industries will be contacted in order to familiarize them with TPV and to enlist their support in integrating TPV technology into their processes.

Keywords: Thermophotovoltaic, Photovoltaic, GaSb Cells, Ceramic Emitter

99. **LOST FOAM CASTING QUANTIFIER PROGRAM**
$64,042
DOE Contact: Roxanne Danz (303) 275-4706
Industrial Analytics Corporation Contact: Graham V. Walford (865) 482-8424

The objective of this grant is to build a prototype of a production floor machine and demonstrate it use in a casting improvement program with a major industry partner. Industrial Analytics Corporation is a product and services business engaged in the development and marketing of non-destructive testing and inspection equipment and analysis services for the manufacturing industry. The industry currently relies on visual inspection of foam patterns pieces to determine quality. The casting of inferior foam patterns results in defective castings. Each defective casting represents a waste of energy. The “Lost Foam Casting Quantifier Program” sets objectives, measurable standards, and verifies them using measured data, the properties of foam patterns may be optimized, production yield can be maximized, quality can be assured, and disputes minimized.

Keywords: Metal Casting, Lost Foam Casting, Non-Destructive Testing

100. **A HOT EYE™ BASED COORDINATE MEASURING MACHINE FOR THE FORGING INDUSTRY**
$130,226
DOE Contact: Roxanne Danz (303) 275-4706
OG Technologies Contact: Tzyy-Shuh Chang (734) 769-8500

The objective of this project is to develop a 3 dimensional measurement system for the domestic forging industry based on HotEye. This technology will allow high definition camera to accurately image a red hot object. The project marries conventional Coordinate Measurement Machine “CMM” technology to HotEye technology to permit the accurate measurement of forged parts while they are at high temperature. Being able to take such measurements will dramatically reduce the amount of scrap produced by the domestic forging industry. This industry wastes a significant amount of energy because of the high rate of scrap it produces.

Keywords: HotEye, Forging, Coordinate Measurement Machine

101. **DEVELOPMENT OF A HIGH-FREQUENCY EDDY-CURRENT SEPARATOR**
$126,942
DOE Contact: Roxanne Danz (303) 275-4706
EMPS Corporation Contact: Stephen Smoot (801) 582-7600

The objective of this grant is to confirm prior bench scale testing of the high-frequency eddy-current separator through the successful scale-up and test of a prototype-size unit. The engineering prototype will be demonstrated on contaminated foundry sand at the Eriez test facilities in Erie, PA, and on magnesium smut at the Interworld magnesium recovery facility. The initial market study and business plan will be refined based on the results of the prototype unit testing and demonstration.

Keywords: Foundry Sand, Foundries, Separations, Magnesium Smut

102. **INTEGRATED ACOUSTIC KILN MONITOR TO GUIDE ACCELERATED DRYING OF WOOD**
$91,942
DOE Contact: Keith Bennett (303) 275-4905
Perceptron, Inc. Contact: Mark Schafer (610) 832-2100

The objective of this grant is to complete two pre-production prototypes of the Acoustic Kiln Monitor and demonstrate them in a commercial environment. The ultimate goal is to help operators accelerate lumber drying to its optimal endpoint, while minimizing damage to the wood caused by speeding the drying process.

Keywords: Forest Products, Sensors and Controls, Lumber Drying, Kiln Monitor

103. **DEVELOPMENT OF AN ENERGY-SAVING GRAIN DRYING INVENTION**
$41,942
DOE Contact: Keith Bennett (303) 275-4905
Shivvers, Inc. Contact: Steve Shivvers (641) 872-1005

This grant will use computer models for final process design and development of the control system followed by the mechanical design of an integrated grain drying technology. This will lead to a full-scale pre-production unit for final performance testing and commercial demonstration.

Keywords: Agriculture, Grain Drying

104. **SYSTEM FOR DETECTION AND CONTROL OF DEPOSITION IN KRAFT RECOVERY BOILERS AND MONITORING GLASS FURNACES**
$83,942
DOE Contact: Doug Hooker (303) 275-4780
Combustion Specialist, Inc. Contact: George Kychakoff (425) 432-1589

This grant will finish the development of a system to monitor and control deposition on the pendant tubes of recovery boilers and investigate the applicability of the system to utility boilers and glass furnaces.

Keywords: Forest Products, Kraft Recovery Boilers, Sensors and Controls

105. **DEVELOPMENT AND COMMERCIALIZATION OF BIOPULPING**
$174,942
DOE Contact: Doug Hooker (303) 275-4780
Biopulping International, Inc. Contact: Masood Akhtar (608) 231-9484

This grant will confirm prior bench-scale testing of the proposed technology through the successful scale-up and test of the prototype-size in cooperation with a mill. For the first time, we will study the final product made through the mill's paper machine. Additionally, the initial market study and business plan will be refined based on the results of the prototype unit.

Keywords: Forest Products, Pulping, Fungus, Wood Chip Penetration

106. **DEVELOPMENT OF A LOWER pH COPPER FLOTATION REAGENT SYSTEM**
$91,692
DOE Contact: Roxanne Danz (303) 275-4706
Versitech, Inc. Contact: Sharon Young (520) 742-9457

This grant will develop a system of reagents that can allow mill flotation operators to reduce or eliminate the amount of lime that they use. The system would be pilot plant scale tested to identify and solve any problems that are caused anywhere in the flotation circuit. Possible problem areas include froth bed height in the roughers or the cleaners, recovery losses in the cleaners, and tail flocculation. Froth height problems can be overcome by frother modifications. Loss of recovery in the cleaner can be handled by collector modification, while the flocculation of the tailing can be achieved by changing the flocculent.

Keywords: Mining, Copper, Flotation, Collectors, Flocculation

107. **MINIATURE, INEXPENSIVE, AMPEROMETRIC OXYGEN SENSOR**
$126,942
DOE Contact: Doug Hooker (303) 275-4780
CeramPhysics, Inc. Contact: William Lawless (614) 882-2231

The purpose of this project is to bring a small, inexpensive, amperometric oxygen sensor to the commercialization stage for both combustion control and breathing-oxygen applications. Initial work has resulted in the manufacture of several batches of sensors. These sensors are currently being placed in several industrial applications for testing.

Keywords: Sensors and Controls, Oxygen Sensor, Combustion, Transportation

108. **EXTREMELY COMPACT AND EFFICIENT CHEMICAL REACTOR**
$139,942
DOE Contact: Doug Hooker (303) 275-4780
Mesoscopic Devices, LLC Contact: Jerry Martin (303) 446-6968

This grant will develop a catalytic heat exchanger reactor for use in the chemical, utility and transportation industries. Our specific objective for the proposed project is to confirm and refine analytical models by fabricating and testing a fuel reformer that can be used to generate syngas from liquid hydrocarbon fuels. In this project, we will upgrade analytical models for the heat and mass transfer within the reactor, develop fabrication techniques for producing the reactors in several sizes at commercially viable costs, select catalysts for the reforming operation, build and test reformer prototypes and refine our initial market study based on the results of the prototype fabrication and testing. Tests of the complete reactor will demonstrate its ability to start rapidly, follow changing loads and produce a high quality syngas or hydrogen stream. The output of the project will be performance measurements for a complete fuel reformer capable of supplying reformate to solid oxide fuel cells, or, through a membrane hydrogen separator, to PEM fuel cells, as well as a market analysis to guide the commercialization after prototype demonstration.

Keywords: Syngas, Chemicals, Fuel Reformer, Catalytic Heat Exchanger

109. **HIGH THROUGHPUT VACUUM PROCESSING FOR INNOVATIVE USES OF GLASS**
$76,942
DOE Contact: Roxanne Danz (303) 275-4706
AVA Technologies, Inc. Contact: Kurt Barth (970) 491-8411

In this grant, a system with HPD sources and glass heaters for processing 1 x 1 foot substrates will be developed and tested. A belt arrangement similar that used in the current AVA prototype will be used for transporting substrates from one process module to the next. There will be up to seven processing stations in the vacuum chamber. The processing of complete photovoltaic devices will also be tested.

Keywords: Glass, Photovoltaic Panels, High Pressure Deposition

110. **ENERGY CONSERVATION WASTE REDUCTION IN THE PROCESSING OF SOFT (UNFIRED) CERAMIC PARTICLES VIA DYNAMIC CYCLONE CLASSIFICATION**
$106,160
DOE Contact: Roxanne Danz (303) 275-4706
InnovaTech, Inc. Contact: Steve Crouch (919) 881-2197

This grant will confirm prior bench-scale DCC performance through the successful scale-up and testing of a full-sized (2 ton/hr) Beta prototype. A market study and business plan will be produced based on scale-up costs and performance.

Keywords: Ceramics, Dynamic Cyclone Classification, Soft Ceramic Particles

NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE^3)
DOE Contact Lisa Barnett (202) 586-2212

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

111. **DEMONSTRATION OF A THREE-PHASE ROTARY SEPARATOR TURBINE**
$0[1]
DOE Contact: Chris Cockrill (816) 873-3299
Douglas Energy Co. Contact: Lance Hays (714) 524-3338
CA Energy Commission Contact: Dennis Fukumoto (916) 653-6222

Douglas Energy and the CA Energy Commission will demonstrate a newly developed compact separator for the petroleum industry which utilizes previously wasted process energy to generate power and separate gas, oil, and water. This technology, to be demonstrated at a Chevron 15,000 barrel per day facility, will substantially improve the efficiency and productivity of high-pressure offshore oil and gas drilling operations.

Keywords: Oil and Gas Production, Hydrocarbon Separation, Petroleum

112. **PRECISION IRRIGATION TECHNOLOGIES FOR THE AGRICULTURAL INDUSTRY**
$0[1]
DOE Contact: Jack Jenkins (303) 275-4805
CO Office of Energy Management Contact: Olga Ehrlich (303) 894-2383
CO Corn Growers Admin. Committee Contact: Harold Smedley (303) 674-5465

The CO Office of Energy Management and the Colorado Corn Administrative Committee will demonstrate and

[1]Prior year funding

commercially validate a unique site specific technology called "Accu-Pulse." It includes a software-based data collection system that analyzes water, nutrients, vegetative material, and pests in individual sub-areas within a larger field so they can be effectively managed for maximum production and/or minimal inputs of water, fertilizers and pesticides. This will reduce waste, save water and energy, and enable farmers to remain economically competitive.

Keywords: Agriculture, Precision Irrigation

113. **ENERGY CONSERVING TOOL FOR COMBUSTION DEPENDENT INDUSTRIES**
$0[1]
DOE Contact: Scott Hutchins (617) 565-9765
CT Bureau of Waste Management Planning & Standards Division Contact: Lynn Stoddard (860) 424-3236
AFR Contact: James Markham (860) 528-9806

CT Bureau of Waste Management Planning & Standards Division and Advanced Fuel Research (AFR) will demonstrate a new, portable, low-cost, energy-efficient multi-gas analyzer for industries utilizing combustion boiler and turbine systems. This state-of-the-art combustion-tuning tool saves substantial fuel, reduces emissions, and validates pollution abatement/control technology.

Keywords: Combustion Tuning, Multi-Gas Analyzer, Boiler, Turbine System

114. **ENERGY-SAVING REGENERATION OF HYDROCHLORIC ACID PICKLING LIQUOR**
$0[1]
DOE Contact: Scott Hutchins (617) 565-9765
CT Bureau of Waste Management Planning & Standards Division Contact: Lynn Stoddard (860) 424-3236
Green Technology Contact: Doug Olsen (914) 855-0331

CT Bureau of Waste Management Planning & Standards Division and Green Technology Group will demonstrate an innovative technology that regenerates spent hydrochloric acid from steel pickling, that results in 95 percent energy savings, 52 percent cost savings, and 91 percent reduction in CO_2 over conventional technologies. This process generates no wastewater or residual waste, and produces significant operating and capital cost savings in addition to major energy savings.

Keywords: Hydrochloric Acid Recovery, Pickle Liquor, Galvanizing

115. **SUPERCRITICAL FLUID PURIFICATION OF COMBI-CHEM LIBRARIES**
$0[1]
DOE Contact: Joe Barrett (215) 656-6957
DE Economic Development Office Contact: Robert Propes (302) 672-6848
Berger Instruments Contact: Ken Klein (302) 266-8201

DE Economic Development Office and Berger Instruments will demonstrate an innovative Scale Supercritical Fluid Chromatograph (SFC) that purifies combinatorial chemistry compound libraries at 20 to 100 times the rate of current systems. This innovation makes it economically feasible for pharmaceutical companies to purify hundreds of thousands of compounds per year with 90 percent recovery and 95 percent purity, while reducing both energy consumption and solvent waste by more than 90 percent, compared to current methods. SFC has the industry-wide potential of saving 4 million gallons of chemical waste, and 590 megawatt-hours of electricity per year.

Keywords: Pharmaceuticals, Combinatorial Chemistry, Compound Purification

116. **FULL-SCALE 100 TON/HR DEMONSTRATION OF MAGNETIC ELUTRIATION TECHNOLOGY FOR CLEAN AND EFFICIENT PROCESSING OF IRON ORE**
$0[1]
DOE Contact: Brian Olsen (312) 353-8579
MN Dept. Public Service Contact: Jeremy DeFiebre (651) 297-1221
5R Research Contact: John McGaa (651) 730-4526

MN Dept. Public Service and 5R Research Inc. will demonstrate an improved mineral processing technology known as "magnetic elutriation" which increases selectivity when weakly-magnetic tailings are separated from magnetic iron ores. This patented process produces yields of 99 percent magnetic iron recovery, while eliminating the need for chemicals used in conventional separation practices. Industry wide, this innovation will reduce chemical use by 1700 tons and save 170 GWhrs of electrical energy each year.

Keywords: Mining, Magnetic Elutriation, Mineral Processing

117. **PRODUCTION-SCALE COMMERCIAL DEMONSTRATION OF A VANADIUM CARBIDE COATING PROCESS FOR ENHANCING WEAR RESISTANCE OF METALS IN STEEL AND OTHER MANUFACTURING INDUSTRIES**

[1]Prior year funding

$491,840
DOE Contact: Joe Barrett (215) 656-6957
PA Dept. of Environmental Protection Contact:
Calvin Kirby (717) 783-9981
Metlab-Potero Contact: James Coneybear
(215) 233-2600

The PA Dept. of Environmental Protection and Metab-Potero will design, install, optimize and operate a production scale system for commercial application of a vanadium carbide coating process. In addition to this, the program will develop and maintain a database for performance of the VC coatings used in different industrial applications. The database will include best practices for applications that will enable the industry to select and apply the optimum coatings.

Keywords: Vanadium Carbide, Steel, Wear Resistance, Surface Hardening

118. **COMMERCIAL DEMONSTRATION OF AN IMPROVED MAGNESIUM THIXOMOLDING PROCESS**
$484,000
DOE Contact: Brian Olsen (312) 886-8579
State of Michigan, Energy Division Contact:
John Trieloff (517) 241-6224
Thixomat, Inc. Contact: Ray Decker
(734) 995-5550

State of Michigan, Energy Division and Thixomat, Inc. will demonstrate the improved Thixomolding Process (semi-solid metal molding), rather than a conventional die-casting foundry operation with the objective to reduce energy usage by 50 percent, reduce scrap recycling by 50 percent, eliminate the application of global warming gas, SF_6, eliminate waste slag and dross with their disposal problems, provide a worker/environmentally friendly process, that can be integrated into an automated manufacturing cell to produce metal and metal/plastic assemblies, and cut costs by more than 20 percent.

Keywords: Magnesium Alloy Molding, Semi-Solid Molding, Net Shape, Scrap Reduction

119. **IMPROVEMENT OF THE LOST FOAM CASTING PROCESS**
$525,000
DOE Contact: Scott Hutchins (617) 565-9765
NYSERDA Contact: Dana Levy (518) 862,1090
GM Contact: Charles Gough (248) 857-2841

NYSERDA and General Motors at Massena, New York, will evaluate and improve the Lost Foam Casting Process by applying recently developed measurement tools related to characterization of dried coating thickness and pore size distribution, improved understanding of rheology of coatings, and the ability to more accurately measure the size and shape of sand as it relates to the casting process.

Keywords: Lost Foam Casting, Metal Casting, Scrap Reduction, Sand Casting

120. **SUPPORT INSPECTION: A METHOD OF INSPECTING ON-STREAM PROCESS PIPING AT SUPPORT AREAS**
$474,994
DOE Contact: Jack Jenkins (303) 275-4805
Texas Natural Resource Conservation
Commission Contact: Jeff Voorhis
(512) 239-3178
Tubular Ultrasound Contact: David Siverling
(713) 426-1072

TNRCC and Tubular Ultrasound will demonstrate to the petrochemical industry the first commercial system to quantify the remaining wall thickness of on-stream piping at pipe supports. The first Support Inspection system demonstration will be used for a series of full-scale commercial demonstrations, evaluations, and certifications at world-class domestic petrochemical facilities.

Key words: Pipe Support Inspection, Petrochemical, Ultrasound

121. **THE FLEX-MICROTURBINE FOR PECAN WASTE: ELECTRICITY AND HEAT IN A NUTSHELL**
$523,395
DOE Contact: Chris Cockrill (816) 873-3299
Flex Energy Co. Contact: Edan Prabhu
(949)-380-4899
AZ Dept. of Environmental Quality Contact:
Kathy Charney (602) 207-2254

AZDEQ and Flex Energy will demonstrate that the Flex-Microturbine will run on pecan shells, that the Flex-Microturbine can consume this residue cost-effectively and cleanly displacing expensive electricity, and the waste heat is capable of drying and pasteurizing the nuts.

Keywords: Micro-Turbine, Low Btu Gas, Pecan Shells, Nut Orchard Processing

122. **PRESSURIZED OZONE MEMBRANE ULTRAFILTRATION METHODOLOGY FOR TDS REMOVAL IN PAPER MILL PROCESS WATER FOR ENERGY SAVINGS, PRODUCTION EFFICIENCY, AND ENVIRONMENTAL BENEFITS**
$525,000
DOE Contact: David Godfrey (404) 562-0568
Linpac Paper Contact: Joe Gasperetti (864) 463-9090
SC Energy Office Contact: Jean-Paul Gouffray (803) 737-8030

The SC Energy Office and Linpac will demonstrate the pressurized ozone membrane ultrafiltration system, from the prototype sized units, to a production scale commercial demonstration size unit. The project will show that TDS removal can be conducted efficiently and create energy, waste, and economic savings.

Keywords: Total Dissolved Solids, Paper Mill, Pressurized Ozone Membrane Ultrafiltration, Process Water

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 2001
OFFICE OF TRANSPORTATION TECHNOLOGIES - GRAND TOTAL	$37,985,000
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES	$23,410,000
TRANSPORTATION MATERIALS PROGRAM	$19,805,000
AUTOMOTIVE PROPULSION MATERIALS	$3,355,000
Technical Project Management	310,000
Low-cost, High Energy Product Permanent Magnets	310,000
Characterization of Permanent Magnets	50,000
Carbon Foam Thermal Management Materials for Electronic Packaging	175,000
High-temperature Capacitors for PNGV Power Electronics	220,000
Mechanical Reliabililty of Electronic Ceramics and Electronic Ceramic Devices	125,000
Microwave-regenerated Diesel Engine Exhaust Particulate Filter Technology	400,000
Rapid Surface Modifications of Aluminum Engine Block Bores for Weight Reduction	175,000
Material Support for Nonthermal Plasma Diesel Engine Exhaust Emission Control	200,000
Carbon Composite Bipolar Plates for PEM Fuel Cells	200,000
Cost-effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	200,000
Low-friction Coatings for Fuel Cell Air Compressors	175,000
Microstructural Characterization of PEM Fuel Cells	200,000
Nanopore Inorganic Membranes as Electrolytes in Fuel Cells	215,000
Inorganic Polymer Electrolyte Membrane Electrode/support Development	75,000
Metallized Bacterial Cellulose Membranes in Fuel Cells	200,000
Carbon Foam for Radiators for Fuel Cells	125,000
LIGHTWEIGHT VEHICLE MATERIALS	$16,450,000
Low-cost High Performance Wrought Aluminum Components For Automotive Applications	500,000
Low-cost High Performance Cast Light Metals for Automotive Applications	1,200,000
Advanced Materials and Processes for Automotive Applications	800,000
Technology Assessment and Evaluation	1,600,000
Advanced Joining	900,000
High Strain Rate Deformation of Materials	400,000
Reinforced Composite Materials-joining, Durability and Enabling Technologies	2,000,000
USAMP Cooperative Agreement	3,400,000
Development of Low Cost Carbon Fiber	3,000,000
Development of Low-cost Lightweight Metals and Alloys	300,000
Recycling	500,000
Structural Reliability of Lightweight Glazing Alternatives	350,000
High Rate Processing Technologies for Composite Materials	1,500,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2001
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES (continued)	
ELECTRIC DRIVE VEHICLE TECHNOLOGIES	$3,605,000
ADVANCED BATTERY MATERIALS	$3,605,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,000,000
Carbon Materials	110,000
Optimization of Anodes for Li-Ion Batteries	240,000
Non-Carbonaceous Materials	130,000
Novel Materials	40,000
Novel Cathode Materials	90,000
New Cathode Materials	90,000
Novel Cathode Structures	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,250,000
Materials Characterization Using X-Ray Diffraction and Chemical Analysis	125,000
Research on Lithium-Ion Polymer Batteries Utilizing Low Cost Materials	205,000
Highly Conductive Polyelectrolyte-Containing Rigid Polymers	60,000
Electrolyte Additives	100,000
Development of Non-Flammable Electrolytes and Thermal Characterization	90,000
Non-Flammable Electrolytes	90,000
Electrode Surface Layers	280,000
Synthesis and Characterization of Electrodes	190,000
EQCM Studies of the SEI on Carbon Anodes	110,000
MATERIALS STRUCTURE AND COMPOSITION	$650,000
R & D for Advanced Lithium Batteries	320,000
Composite Polymer Electrolytes for Lithium and Lithium-Ion Batteries	90,000
Structure and Characterization of Materials	120,000
Interfacial and Reactivity Studies	120,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$705,000
Cell Fabrication and Testing	300,000
Modeling of Lithium/Polymer Electrolytes	70,000
Improved Electrochemical Models	240,000
Failure Mechanisms in Li-Ion Systems: Design of Materials for High Conductivity and Resistance to Delamination	65,000
Thermal Modeling of Li Batteries	30,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2001
OFFICE OF HEAVY VEHICLE TECHNOLOGIES	$14,575,000
HEAVY VEHICLE MATERIALS TECHNOLOGY	$14,575,000
HIGH STRENGTH WEIGHT REDUCTION MATERIALS	$8,975,000
Design, Analysis and Development of Lightweight Frames for Truck and Bus Applications	1,350,000
Development of Advanced Casting Technologies for Production of High Integrity Truck Components	1,200,000
Advanced Forming Technologies for Lightweight Alloys	700,000
Development of Carbon Monoliths for Safe, Low Pressure Adsorption, Storage, and Release of Natural Gas	600,000
Improved Materials for Heavy Vehicle Brake and Friction Applications	400,000
High Conductivity Carbon Foams for Thermal Management	125,000
Advanced Joining Technology Development	250,000
Development of Advanced Materials for Heavy Vehicle Applications	1,500,000
Implementation of Lightweight Materials in Heavy Vehicle Structural Applications	1,550,000
Technology Assessment and Evaluation	1,300,000
HIGH TEMPERATURE MATERIALS LABORATORY	$5,600,000
The High Temperature Materials Laboratory User Program	5,600,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies seeks to develop, in cooperation with industry, advanced technologies that will enable the U.S. transportation sector to be energy efficient, shift to alternative fuels and electricity and minimize the environmental impacts of transportation energy use. Timely availability of new materials and materials manufacturing technologies is critical for the development and engineering of these advanced transportation technologies. Transportation Materials Technologies R&D is conducted by the Office of Advanced Automotive Technologies (OAAT) and the Office of Heavy Vehicle Technologies (OHVT) to address critical needs of automobiles and heavy vehicles, respectively. These activities are closely coordinated between the two offices to ensure non-duplication of efforts. Another important aspect of these activities is the partnership between the Federal government laboratories and U.S. industry, which ensures that the R&D is relevant and that federal research dollars are highly leveraged.

Within OAAT, the bulk of the materials R&D is carried out through the Transportation Materials Technologies program, with additional specialty materials R&D in the Electric Drive Vehicle Technologies program. The Transportation Materials Technologies program develops: a) Automotive Propulsion Materials to enable advanced propulsion systems for hybrid vehicles and b) Automotive Lightweight Vehicle Materials to reduce vehicle weight and thereby decrease fuel consumption. The program seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis and powertrain are critical to attaining the challenging performance standards for advanced automotive vehicles. The DOE contacts are Nancy Garland (202) 586-5673, for automotive propulsion materials and Joseph Carpenter (202) 586-1022, for automotive lightweight vehicle materials. The Electric Vehicle R&D program includes the support of Advanced Battery Development for electric and hybrid vehicle applications. The DOE contact is Ray Sutula (202) 586-8064.

The Heavy Vehicle Materials Technology program focuses on two areas: a) Heavy Vehicle Propulsion System Materials and b) High Strength Weight Reduction Materials. In collaboration with U.S. industry and universities, efforts in propulsion system materials focus on the materials technology critical to the development of the low emission, 55 percent efficient (LE-55) heavy-duty and multi-purpose Diesel engines, such as: manufacturing of ceramic and metal components for high-efficiency turbocharger and supercharger; thermal insulation, for reducing engine block cooling, lowering ring-liner friction and reducing wear; high-pressure fuel injection materials; and exhaust after treatment catalysts and particulate traps. In the area of high strength weight reduction materials, energy savings from commercial trucking is possible with high strength materials which can reduce the vehicle weight within the existing envelope so as to increase payload capacity and thereby reducing the number of trucks needed on the highways. Increased safety can be obtained by new brake materials and by incorporating highly shock absorbent materials in truck structures for improved control and crashworthiness. The DOE contact is Sid Diamond (202) 586-8032.

The High Temperature Materials Laboratory (HTML) at the Oak Ridge National Laboratory is a modern research facility that houses in its six user centers, a unique collection of instruments for characterizing materials. It supports a wide variety of high-temperature ceramics and metals R & D. The HTML enables scientists and engineers to solve materials problems that limit the efficiency and reliability of advanced energy-conversion systems by providing access to sophisticated state-of-the-art equipment (which few individual companies and institutions can afford to purchase and maintain) and highly trained technical staff. The DOE contact is Sid Diamond (202) 586-8032.

OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES

TRANSPORTATION MATERIALS PROGRAM

AUTOMOTIVE PROPULSION MATERIALS

123. **TECHNICAL PROJECT MANAGEMENT**
$310,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556

The objective of this effort is to assess the ceramic technology needs for advanced automotive heat engines, formulate technical plans to meet these needs and prioritize and implement a long-range research and development program. An additional task in FY 2001 was to organize and host the 2001 Fuel Cell Laboratory R&D Review that was held at Oak Ridge National laboratory from June 6-8, 2001.

Keywords: Advanced Heat Engines, Alloys, Automotive Applications, Carbon, Coordination, Metals, Management, Structural Ceramics

124. **LOW-COST, HIGH ENERGY PRODUCT PERMANENT MAGNETS**
$310,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: T. M. Mulcahy (630) 252-6141

The objective of this work is to develop a low-cost process for the fabrication of high-strength NdFeB permanent magnets to enable significant size and weight reductions of traction motors for hybrid electric vehicles. A facility was established at Argonne National Laboratory for pressing permanent magnets in the high fields (9 T) of a superconducting solenoid. The solenoid better aligns the magnetic domains of NdFeB powder during pressing into green compacts. The energy product (MGOe) and remnant field Br(kG) of magnets produced in this facility showed a strong dependence on the magnitude of the alignment field H(T). Energy products that were within 10 percent of the theoretical maximum were achieved by optimizing batch-mode alignment/pressing of cylindrical axial-die-pressed PMs in a 9-Tesla (T) superconducting solenoid. Energy product improvements of 15 percent over commercial magnets resulted when powder-filled dies were inserted into and pressed compacts were removed from an active (always on) superconducting solenoid.

Keywords: NdFeB, Permanent Magnets, Superconducting Solenoids, Traction Motors

125. **CHARACTERIZATION OF PERMANENT MAGNETS**
$50,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: E. A. Payzant (865) 574-4472

The purpose of this work is to quantify the relationship between processing parameters and the crystal chemistry and microstructure of NdFeB permanent magnets fabricated at Argonne National Laboratory and by commercial suppliers. The microscopic texture (alignment) of permanent magnets made in the Argonne axial-die press facility was characterized and correlated the alignment with macroscopic magnetic properties.

Keywords: NdFeB, Permanent Magnets

126. **CARBON FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING**
$175,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: J. W. Klett (865) 574-5220

The objective of this work is to collaborate with automotive partners to develop carbon foam heat exchanger and heat sink designs for high-power electronics that dissipate 30 W/cm^2 using conventional cooling fluids. A test facility was used to evaluate the performance of various carbon foam heat sink designs. Novel carbon foam heat sinks were tested that dissipated greater than 30 W/cm^2 at temperatures of less than 60^{o}C with lower cooling flow rates than current designs. Collaborative research with Anteon showed that blind holes successfully reduce the pumping power required while maintaining high heat transfer. Collaborative research with the National Security Agency proved that novel passive cooling systems that utilize evaporative cooling can dissipate greater than 100 W/cm^2 of heat.

Keywords: Carbon Foam, Heat Sinks, Heat Transfer, Power Electronics, Thermal Management

127. **HIGH-TEMPERATURE CAPACITORS FOR PNGV POWER ELECTRONICS**
$220,000
DOE Contact: N. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
SNL Contact: B. A. Tuttle (505) 845-8026

The objective of this work is to develop a high-temperature polymer dielectric film technology that has dielectric properties technically superior to those of aluminum electrolytic dc buss capacitors and is comparable or smaller in size. A plan was developed for large-scale commercialization of polymer film dc buss capacitors with AVX/TPC, GM and Sandia National Laboratory. New polymer film dielectrics were fabricated with five times the energy density of commercial polyphenylene sulfide at 110°C. These films exhibited properties ranging from dielectric constants of from K=6 and DF=0.009 to K=4 and DF=0.002.

Keywords: Capacitors, Dielectrics, Polymer Films, Power Electronics

128. **MECHANICAL RELIABILILTY OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC DEVICES**
$125,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: M. K. Ferber (865) 576-0818

The objectives of this task are to predict and assess the mechanical reliability of electronic devices with emphasis on those used for automotive power electronics (e.g., capacitors) and to correlate the mechanical characterization of polymer film capacitors developed by Sandia National Laboratories (SNL) to the dielectric behavior.
A micro-mechanical test apparatus was fabricated and used to directly measure the strength of small multi-layer ceramic capacitors (MLCCs). An analytical model for predicting residual stresses in MLCCs was developed and applied to explain strength differences in several varieties of 1206 MLCCs. A series of polymer film dielectric samples was received from SNL and characterized using a mechanical properties microprobe.

Keywords: Electronics, Failure Analysis, Life Prediction, Mechanical Properties, Multilayer Capacitors

129. **MICROWAVE-REGENERATED DIESEL ENGINE EXHAUST PARTICULATE FILTER TECHNOLOGY**
$400,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
Industrial Ceramic Solutions Contact: R. Nixdorf (865) 482-7552

The objective of this work is to develop a Diesel Particulate Filter that demonstrates greater than 95 percent capture efficiency and can be regenerated to within 95 percent of the new filter condition with the use of microwave energy. During the year a microwave regeneration system was designed and built that is capable of performing on a PNGV-type diesel engine. The microwave filter system demonstrated 95 percent efficiency on an l.9-L Volkswagen engine in a test cell at Oak Ridge National Laboratory. A similar microwave filter system was installed on a Ford F.250 7.3-L diesel pickup, with full exhaust backpressure and temperature data acquisition, for on-highway testing. The microwave filter system fuel penalty, as calculated from these test results, was an impressively low 0.3 percent.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

130. **RAPID SURFACE MODIFICATIONS OF ALUMINUM ENGINE BLOCK BORES FOR WEIGHT REDUCTION**
$175,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: C. Blue (865) 574-5112

Innovation, rapid, high-density surface modification processes are being used to develop a new, durability-enhancing coating for automotive applications such as aluminum engine block cylinder bores, compressor housings, fuel pumps and sealing surfaces. Coatings were produced by fusing fine WC and Cr_2C_3 particulates in copper- and nickel-based binders directly onto aluminum surfaces using a high-density radiant heating process. Metallography and hardness testing have quantified the quality of this coating.

A pump thrust body presently cast out of 390 aluminum was identified as a component that, because of wear issues, would benefit from a new wear-resistant coating. The development of a plasma-assisted deposition process capable of depositing wear-resistant 390 aluminum onto easily machinable 319 aluminum was completed this year. A pump thrust body presently cast out of 390 aluminum was identified as a component that, because of wear issues would benefit from a new wear-resistant coating. An additional aluminum surface modification application was identified where economical crash triggers are placed in aluminum structures, using selective area heat treatment via arc lamp processing.

Keywords: Aluminum, Cost Reduction, Engines, Hard Coatings, Wear

131. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DIESEL ENGINE EXHAUST EMISSION CONTROL**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: S. D. Nunn (865) 576-1668

The objective of this work is to identify appropriate ceramic materials, develop processing methods and fabricate complex-shaped ceramic components that will be used in Pacific Northwest National Laboratory (PNNL)-designed nonthermal plasma (NTP) reactors for the treatment of diesel exhaust gases. It was concluded that the gelcasting process was probably not amenable to high-volume commercial production and would, therefore, be too costly. Tape-cast ceramic components were fabricated for the PNNL NTP-reactor that were 62 percent lighter than previous components yet had the same active surface area. The ceramic component processing temperature was reduced from 1600 to 850°C, which lowers the fabrication cost and permits the use of readily available silver inks for the electrodes. Trial components were fabricated using the new process and shipped to PNNL for examination.

Keywords: Aftertreatment, Ceramics, Diesel, Gelcasting, Nonthermal Plasma

132. **CARBON COMPOSITE BIPOLAR PLATES FOR PEM FUEL CELLS**
$200,000
DOE Contact: JoAnn Milliken (202) 586-2480
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: T. M. Besmann (865) 574-6852

The purpose of this work is to develop a slurry-molded carbon fiber material with a carbon chemical-vapor-infiltrated (CVI) sealed surface as a bipolar plate. During the year, the process used to fabricate single-sided bipolar plates was modified and improved to permit fabrication of double-sided plates with active surface areas of 100-cm^2. Corrosion testing over a 60-day span revealed little effect on the material-its performance was superior to that of the material supplied by Poco Graphite. The polarization behavior in a cell was determined to be comparable to graphite. The through-thickness thermal conductivity was found to be low; however, the cell behavior was good. A number of double-sided bipolar plates were fabricated and shipped to potential fuel-cell manufacturers for testing and evaluation. The technology was licensed to Porvair Fuel Cell Technology for scale up and manufacturing.

Keywords: Bipolar Plates, Carbon Composites, Fuel Cells, Manufacturing

133. **COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY**
$200,000
DOE Contact: JoAnn Milliken (202) 586-2480
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: M. P. Brady (865) 574-5153

The objective of this work is to develop a titanium-containing bipolar plate alloy that will form an electrically conductive and corrosion-resistant TiN surface layer during thermal nitridation. The alloy must meet DOE cost/performance goals related to the $10/kW bipolar plate target. The nitridation behavior of a series of developmental Ni-Ti and Fe-Ti base alloys with ternary and quaternary-alloying additions was metallographically evaluated. Alloy chemistries/ nitridation conditions were identified that led to the formation of adherent TiN-base surface layers with good corrosion resistance in short-term, 5 percent hydrofluoric acid immersion screenings. A series of model and developmental alloys were delivered to Los Alamos National Laboratory for corrosion testing in simulated PEM fuel cell environments.

Keywords: Bipolar Plates, Coatings, Corrosion Resistance, Fuel Cells, Nitride

134. **LOW-FRICTION COATINGS FOR FUEL CELL AIR COMPRESSORS**
$175,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: G. R. Fenske (630) 252-5190

The objective of this work is to develop and evaluate the friction and wear performance of low-friction coatings for fuel cell air compressor/expander systems. The impact of the near-frictionless carbon (NFC) coating on the scuffing performance of steel surfaces under dry contact condition was evaluated in laboratory bench top tests using a reciprocating sliding-contact configuration. Thrust washer wear tests showed that Argonne's NFC coating reduced friction by about four times and wear rate by two orders of magnitude. A 50 percent reduction in friction was achieved for application in Variex-variable displacement compressor/expander using Hitco C/C composite and anodized aluminum contact pairs.

Keywords: Air Compressors, Carbon, Friction, Near Frictionless Coating, Scuffing, Wear

135. **MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: D. Blom (865) 241-3898

The objectives of this effort are to optimize the catalyst microstructure and distribution in membrane electrode assemblies (MEAs) for low cost and high performance and to understand the effects of microstructure and microchemical composition on the performance and aging characteristics of the fuel cell. A new specimen preparation technique has been developed and demonstrated that produces thin cross-sections of PEM fuel cell MEAs suitable for microstructural and microchemical characterization in a TEM. Negligible performance degradation was observed for the given test conditions over 325 hours of continuous use; however, several microstructural changes have been observed to occur as an MEA ages. An interfacial layer approximately 50-100 nm wide, enriched in sulfur and depleted in fluorine relative to the bulk PEM, has been shown to develop at both the cathode and anode interfaces of the PEM. Coarsening of the platinum catalyst occurred during the aging test.

Keywords: Catalysts, Fuel Cells, Platinum Membrane Electrode Assemblies, TEM Characterization

136. **NANOPORE INORGANIC MEMBRANES AS ELECTROLYTES IN FUEL CELLS**
$215,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
U. of Wisconsin Contact: M. A. Anderson (608) 262-2674

The objective of this work is to develop microporous inorganic membranes of TiO_2, with high proton conductivity that is capable of operating at temperatures above 100°C with minimal water management problems. Inorganic PEMs represent a fundamental departure from the polymer-based PEMs currently used in hydrogen fuel cells. Therefore, fuel cells built using inorganic PEMs will require a significantly different fabrication method. In particular, inorganic PEMs are not free standing, but rather need to be supported on a strong, porous substrate because the membranes are inherently ultra-thin and brittle. Inorganic membranes were developed that demonstrated proton conductivity at temperatures up to 110°C at relative humidities between 13 and 44 percent. A novel method was developed for applying the ceramic sandwich layer to the nickel substrates that may also be useful in other membrane applications.

Keywords: Fuel Cells, Inorganic Membranes, Proton Conductivity, PEM

137. **INORGANIC POLYMER ELECTROLYTE MEMBRANE ELECTRODE/SUPPORT DEVELOPMENT**
$75,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: M. A. Janney (865) 574-4281

The goal of this effort is to develop electrically conducting electrodes/supports and catalytically active ceramic sandwich layers for use in inorganic microporous PEM membranes based on nanoparticles of TiO_2 and Al_2O_3. The materials developed in this project will be used as substrates at the University of Wisconsin for the fabrication of microporous inorganic proton exchange membranes. A process was developed to fabricate electrically conducting, porous nickel materials that will be initially used as substrates. An improved graphite fiber-based substrate/electrode having the requisite chemical compatibility with the PEM environment is being developed to replace the porous nickel. After successful development of the substrates, a second process was devised to deposit microporous titania with carefully controlled particle size and permeability onto the substrate. Sandwich layers of microporous titania on porous nickel were fabricated and shipped to the University of Wisconsin. The nickel/titania sandwich material was found to be an appropriate surface upon which to deposit the nanoparticle membrane.

Keywords: Ceramics, Fuel Cells, Membranes, Titanium Oxide

138. **METALLIZED BACTERIAL CELLULOSE MEMBRANES IN FUEL CELLS**
$200,000
DOE Contact: JoAnn Milliken (202) 586-2480
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: H. O'Neill (865) 574-5004

The objective of this task is to develop low-cost bacterial cellulose membranes with high proton conductivity that is capable of operating at above 120°C with minimal water management problems. The present concept proposes a cellulose matrix secreted by bacteria as a suitable material for PEM fuel cell technology development. The catalyst and electrolyte membrane components of the MEA are constructed using bacterial cellulose, underlining the multifunctional nature of this material. The main impact, at the system level, of a cellulose-based PEM fuel cell is that it will operate at temperatures ≥130°C, circumventing the problems associated with Nafion-based PEM fuel cells. The operation of a bacterial-cellulose-based MEA was demonstrated albeit at low efficiency. Efforts are directed toward increasing efficiency by development of the electrolyte layer, catalyst layer and current collectors.

Keywords: Fuel Cells, Membranes, Bacterial Cellulose, Water Management

139. **CARBON FOAM FOR RADIATORS FOR FUEL CELLS**
$125,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: J. W. Klett (865) 574-5220

The purpose of this work is to develop compact, lightweight and more efficient radiators for fuel-cell-powered vehicles utilizing Oak Ridge National Laboratory's unique, high-conductivity carbon foam. Most air/water heat exchangers, like automobile radiators, exhibit an overall heat transfer coefficient of about 20-30 $W/m^2 \times K$. The initial heat transfer coefficient of a prototype radiator was calculated to be between 3700 and 5400 $W/m^2 \times K$. No appreciable change in heat transfer coefficient was observed over 46,000 thermal cycles between room temperature and 125°C. A proprietary conductive braze was developed for joining the graphite foam to a metallic substrate in a collaborative effort with Materials Research, Inc. This braze has allowed for an increase in the heat transfer, as thermal impedance is greatly reduced or eliminated.

Keywords: Carbon Foam, Heat Exchangers, Heat Transfer, Radiators

LIGHTWEIGHT VEHICLE MATERIALS

140. **LOW-COST HIGH PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
$500,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: LANL, PNNL
Industry Partners: Alcoa

The objectives of this effort are: to evaluate and improve aluminum forming processes for automotive applications; to develop numerical-based analysis tools that can be used to develop and optimize the forming process and predict distortions of multi-element structures.

Keywords: Aluminum, Sheet Forming, Extrusion

141. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$1,200,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Ed Courtright (509) 375-6926
Laboratory Partners: LLNL, ORNL, SNL, INEEL, PNNL, ANL
Industry Partners: USAMP (Ford, GM, Chrysler), LEP (Ford, GM, Chrysler)

The objectives of this effort are: to optimize design knowledge and improve product capability for light-weight, high-strength, cast structural components; to improve the energy efficiency and cost effectiveness of large-scale automotive aluminum die castings by extending die life and reducing die wear; to develop magnesium die casting alloys with improved high temperature properties

Keywords: Aluminum, Magnesium, Cast Metals, Automotive, Die Life, Die Wear, Die Castings

142. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
$800,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: Ames Laboratory, PNNL
Industry Partners: USAMP (Ford, GM, Chrysler), MC-21

The objectives of this effort are: to develop low cost powder metallurgy (PM) manufacturing methods for particle reinforced aluminum (PRA) composite components; to advance PRA machining technology and PRA composite design methodologies; to develop a new low-cost process for the efficient on-site stir-casting of aluminum metal matrix composites suitable for the production of automotive components.

Keywords: Metal Matrix Composites, Powder Metallurgy, Aluminum, Particle Reinforced Aluminum

143. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,600,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
Laboratory Partners: ANL, ORNL, PNNL

The objective of these activities is: to provide assessment of the cost effectiveness of various technologies; to evaluate the ability of the industrial infrastructure to accommodate emerging technologies; to provide guidance to program management as to appropriate investments for R&D funding; and to fund innovative research with small businesses.

Keywords: Cost, Infrastructure, Technical Management

144. **ADVANCED JOINING**
$900,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
Laboratory Partners: LBNL, ORNL, PNNL
University Partners: Kansas State University

The objective of this project is to: develop nondestructive evaluation and testing techniques that are sufficiently fast, robust in manufacturing environment, accurate and cost-effective to be suitable for on-line inspection of automotive structures and to develop and evaluate different joining technologies for dissimilar aluminum alloys and aluminum to steel. In cooperation with the ACC Materials and Joining Working Groups, develop and demonstrate reliable attachment technologies for use in lightweight composite structures for automotive applications and long term durability test methodologies, durability driven design guidelines, joint test methods, non-destructive inspection techniques and material models which can be used in designing automotive components. Specific technology thrust areas include the development of test methods, creep, fracture, fatigue and environmental durability using carbon fiber reinforced composites. This work includes the characterization of bulk adhesives, bolted joints, sheet composite, sheet metals and composite-metal pairs. Models are being developed to simulate the fracture behavior of bonded joints under a wide range of mode mixes and define the fracture envelope. NDE technology is being developed to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white.

Key words: Joining, Dissimilar Materials, NDE, Aluminum, High Strength Steels, Polymer Composites

145. **HIGH STRAIN RATE DEFORMATION OF MATERIALS**
$400,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: AISI

The objective of this project is to develop numerical modeling guidelines in order to realistically assess the influence that the properties of strain rate dependent materials exert in crashworthiness computations.

Key words: Strain Rate, Crashworthiness, Numerical Modeling

146. **REINFORCED COMPOSITE MATERIALS-JOINING, DURABILITY and ENABLING TECHNOLOGIES**
$2,000,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: LLNL, ORNL
University Partners: University of Tennessee, University of Tulsa, University of Michigan, University of California-Santa Barbara, Wayne State University, Stanford University, University of Nottingham.
Industry Partners: USAMP/Automotive Composites Consortium, Dow, Goodrich, Baydur Adhesives

The objective of this effort is to develop enabling technologies necessary for the implementation of advanced structural composites. In cooperation with the ACC Energy Management working group, develop material and component level models for composite materials in high-energy impacts for prediction of passenger safety and optimization of component designs. Composite research is to lead to the development of experimentally-based, durability-driven design guidelines to assure the long-term (15 year) integrity of polymeric composite automotive structures.

Keywords: Polymer, Composites, Fracture, Durability, Automotive, Adhesives, Non-Destrucive Inspection, Environmental Degradation

147. **USAMP COOPERATIVE AGREEMENT**
$3,400,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORO Contact: Mary Rawlins (865) 576-0823
University Partners: University of Tulsa, University of Michigan, University of Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham.
Industry Partners: US Automotive Materials Partnership (DaimlerChrysler, Ford, GM), Goodrich, Baydyr Adhesives, Dow, Westmoreland, EKK, Entelechy, American Foundryman's Society, Mascotech, Stackpole Ltd., Valimet, Aluminum consultant's Group.

The objectives of this project are to define and conduct vehicle related R&D in materials and materials processing. Projects include Structural Cast Magnesium Development, Hydroforming of Aluminum Tubes, Powder Metallurgy of Particle Reinforced Aluminum, Design and Product Optimization of Cast Light Metals, Warm Forming, Enhanced Forming of High Strength Steels, P4 Preforming, ACC Focal Project III, high rate composite processing, *composite energy management* and High Volume Processing of Composites. Projects are conducted by multi-organizational teams involving USAMP members, automotive suppliers, universities and private research institutions.

Keywords: Polymer Composites, Aluminum, Magnesium, Free Machining Steel, Glass Fiber Preforming, Adhesive Bonding, Slurry Preforming, Powder Metallurgy, MMC, Rapid Prototyping, NDT, Automotive, Composite Processing

148. **DEVELOPMENT OF LOW COST CARBON FIBER**
$3,000,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL
University Partners: Clemson University, Virginia Technological University, Penn State University, Michigan State University

Industry Partners: USAMP/Automotive Composites Consortium, AKZO Fortafil Fibers, Amoco Cornerstone Technologies, North Carolina State University, Westvaco, Hexcel Corporation

The objective is to conduct materials research to lead to the development of low cost carbon fiber for automotive applications. Research includes investigation of alternate energy deposition methods and alternate precursors for producing carbon fiber as well as the development of improved thermal processing methods and equipment for fiber manufacture. This work examines the fiber architecture and manufacturing issues associated with carbon fiber usage to take advantage of this material's high strength and modulus while minimizing the effects of its low strain to failure. The ultimate goal of this effort is to reduce the cost of commodity grade carbon fiber to $3-5 per pound.

Keywords: Polymer, Composites, Carbon Fiber, Durability, Low Cost Carbon Fiber, Precursor, Carbon Fiber Processing, Microwave Energy

149. **DEVELOPMENT OF LOW-COST LIGHTWEIGHT METALS AND ALLOYS**
$300,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Russ Jones (509) 376-4276
Laboratory Partners: PNNL
Industry Partners: Alcoa, EIMEx, LLC/Boston University, International Titanium Powders, Plasma Quench Titanium Incorporated

The objective of this work is to develop technologies for lowering the cost of primary light metals. Technologies which offer potential to produce sufficient quantities of raw materials for automotive use at substantially reduced cost will be investigated. Efforts include: demonstration of the proof-of principle for the direct reduction of Mg from its oxide using an oxygen ion-conductiong membrane electrolytic process and development of commercial titanium powder production using continuous, molten salt processing.

Keywords: Primary Metal, Low Cost, Reduction Technologies, Magnesium, Titanium

150. **RECYCLING**
$500,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
ANL Contact: George Fenske (630) 252-5190
Laboratory Partners: ANL
Industry Partners: Vehicle Recycling Partnership

The objectives of this effortare: to investigate cost-effective technologies for recycling polymer composites; and to establish priorities for advanced recycling initiatives and provide technical oversight to ensure that priority goals and objectives are accomplished..

Keywords: Recycle, Scrap, Sorting

151. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$350,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: M. A. Khaleel (509) 375-2438
Laboratory Partners: PNNL
Industry Partners: Visteon

The objective of this project is to develop numerical modeling and simulation tools to evaluate the structural behavior and reliability of lightweight, thin glazing designs .

Keywords: Glazing, Structural Reliability

152. **HIGH RATE PROCESSING TECHNOLOGIES FOR COMPOSITE MATERIALS**
$1,500,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
PNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: ORNL, PNL
Industry Partners: USCAR (DaimlerChrysler, Ford, General Motors), Delphi. MASCOTech, Budd Corporation, Enginuity

Develop technologies to cost effectively process composite materials into automotive components, integrate these technologies into demonstration projects that display cost effective use of composites that can be manufactured in automotive factories, develop advanced vehicle system designs based on composite materials to both define future research needs and demonstrate the technical and economic viability of developing technologies.

Keywords: Automotive, Composite, High Rate Processing, Focal Project Design, Thermoplastic Forming

ELECTRIC DRIVE VEHICLE TECHNOLOGIES

ADVANCED BATTERY MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

153. **CARBON MATERIALS**

$110,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
K. Kinoshita (510) 486-7389

The objectives of this project are to investigate the critical parameters that control the reversible intercalation of Li in carbonaceous materials and to identify a low-cost carbon (<$10/kg) for negative electrodes in Li-ion batteries for electric and hybrid vehicles. A chemical procedure to purify natural graphite that is lower cost than thermal purification processes was developed in collaboration with Hydro-Québec. Optimizing the chemical composition to produce purified graphite has not been completed.

Keywords: Carbon Electrode, Li-Ion Batteries

154. **OPTIMIZATION OF ANODES FOR LI-ION BATTERIES**
$240,000
DOE Contact: Ray Sutula (202) 586-8064
University of Michigan Contact: G. A. Nazri
(810) 986-0737

The objective of this project is to investigate the chemical and electrochemical and safety aspects of carbonaceous anodes used in Li-ion batteries and to identify the reaction products that form during charge/discharge cycling of Li-ion cells. New electrically conductive polymers have been prepared for use as a simultaneous binder/artificial passive layer (SEI). The polymers feature a conjugated backbone and pendant groups that are anticipated to enhance Li ion conductivity, decrease the reactivity of the carbon/electrolyte interface, and decrease the cell impedance.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Carbon Electrode

155. **NON-CARBONACEOUS MATERIALS**
$130,000
DOE Contact: Ray Sutula (202) 586-8064
Argonne National Laboratory Contact:
M. M. Thackeray (630) 252-9183

The overall objective of this task is to develop and characterize non-carbonaceous anode materials for high-energy rechargeable Li batteries for EVs and hybrid EVs. The specific objective of the research effort is to identify materials that are inherently safer than carbon-based electrodes (particularly when subjected to overcharge conditions at elevated temperature) without compromising capacity, rate capability and cycle life. Early results show that substituted $Cu_{6-x}M_xSn_{5-x}N_x$ (M is a transition metal and N is a main group metal and Cu_2Sb electrodes) electrodes deliver a slightly lower capacity (~150 mAh/g) than Cu_6Sn_5 electrodes, but show excellent cycling stability in the tests that have been conducted thus far (14 cycles).

Keywords: Non-Carbon Electrodes, Rechargeable Batteries

156. **NOVEL MATERIALS**
$40,000
DOE Contact: Ray Sutula (202) 586-8064
State University of New York Binghamton Contact:
M. S. Whittingham (607) 777-4623

The objective of this project is to identify alternative electrode materials for carbon anodes that are safer and compatible with manganese oxide cathodes and the associated electrolyte. Studies of the oxides based on manganese and iron were completed. The results indicate that these materials have insufficient capacity at a potential of interest (about 1 volt) for use as a practical negative electrode.

Keywords: Non-Carbon Electrodes, Rechargeable Batteries

157. **NOVEL CATHODE MATERIALS**
$90,000
DOE Contact: Ray Sutula (202) 586-8064
Argonne National Laboratory Contact:
M. M. Thackeray (630) 252-9183

The objective of this project is to find lower-cost and higher-capacity cathodes for rechargeable lithium EV batteries than the presently available $LiCoO_2$, while retaining their positive attributes of high cycle life, good electronic conductivity and structural stability. The specific objective of this research will be to identify new transition metal oxide cathode materials, particularly those based on Mn, that offer enhanced behavior in Li-ion and Li/polymer cells. Layered and a-MnO_2 electrodes were synthesized for Li-polymer cell applications. The electrochemical capacity of the electrode improves on cycling, yielding approximately 145 mAh/g after 4 cycles.

Keywords: Intercalation Electrodes, Rechargeable Batteries

158. **NEW CATHODE MATERIALS**
$90,000
DOE Contact: Ray Sutula (202) 586-8064
State University of New York Binghamton Contact:
M. S. Whittingham (607) 777-4623

The objective of this project is to investigate the formation of stabilized manganese oxides, to characterize them structurally and in electrochemical cells. The formation of the vanadium pillared layered manganese dioxides at lower temperatures was investigated. It was observed that the same phase is formed as low as 80˚C, but it is less crystalline. Electrochemical evaluation is underway.

Keywords: Intercalation Electrodes, Rechargeable Batteries

159. **NOVEL CATHODE STRUCTURES**
$300,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact: M. M. Doeff (510) 486-5821

The objective of this project is to develop low-cost cathodes based on manganese oxides and lithium iron phosphates having electrochemical characteristics (e.g., cycle life, energy and power densities) consistent with the goals of the USABC and/or PNGV. A cathode material referred to as "$Li_{1.02}Al_{0.25}Mn_{1.75}O_{3.98}S_{0.02}$" was synthesized by a sol-gel technique reported in the literature and by a solid-state method. Li/1M $LiPF_6$, EC-DMC/$Li_{1.02}Al_{0.25}Mn_{1.75}O_{3.98}S_{0.02}$ cells discharge about 80 mAh/g on the 4-V plateau at C/4 rate and cycle with a slow capacity loss. When cycled over both the 4- and 3-V plateaus, cells discharge about 130 mAh/g at C/8 rate, with rapid capacity fade, in contrast to published reports.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR CHARACTERIZATION OR TESTING

160. **MATERIALS CHARACTERIZATION USING X-RAY DIFFRACTION AND CHEMICAL ANALYSIS**
$125,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact: T. J. Richardson (510) 486-8619

The objective of this project is to accelerate the evaluation of electrode materials by structural characterization of active components as received (or synthesized), following cell disassembly, and *in situ* during cycling. No new phases were found in electrodes taken from cycled commercial Li-ion batteries examined by X-Ray diffraction.

Keywords: Electrode Characterization, X-Ray Analysis, Phase Composition

161. **RESEARCH ON LITHIUM-ION POLYMER BATTERIES UTILIZING LOW COST MATERIALS**
$205,000
DOE Contact: Ray Sutula (202) 586-8064
Hydro-Québec Contact: K. Zaghib (450) 652-8019

The focus of this task is to fabricate Li-ion polymer cells (4 cm^2 area) using cell chemistries proposed by DOE. Cells will be sent to LBNL for testing. Samples of cross-linkable polymers based on polyether were prepared: the first one had an over coating of Celgard membrane (8μm), and the second one is a freestanding polymer-type film of 20 μm thickness. The physicochemical and electrochemical characterization of low-cost $LiFePO_4$ was completed.

Keywords: Li-Ion Polymer Batteries, Low Cost Materials

162. **HIGHLY CONDUCTIVE POLYELECTROLYTE-CONTAINING RIGID POLYMERS**
$60,000
DOE Contact: Ray Sutula (202) 586-8064
Northwestern University Contact: D. F. Shriver (847) 491-5655

The objective of this project is to synthesize and test a new class of rigid polymer electrolytes for rechargeable Li and Li-ion batteries. A polysulfone-based polymer electrolyte was synthesized that had a conductivity of approximately $5x10^{-6}$ S/cm at room temperature, which is lower than anticipated. However, the polysulfone-salt complex was much more stable toward a lithium anode

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolyte

163. **ELECTROLYTE ADDITIVES**
$100,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact: K. Kinoshita (510) 486-7389

The primary objective is to identify chemical additives that improve the safety of nonaqueous electrolytes for Li-ion batteries by stabilizing the SEI layer on carbon. Electrochemical studies of carbon electrodes in EC/DMC electrolyte containing organic bases such as pyrrole and pyridine were initiated. The current-potential profiles of graphite electrodes (Gen 2) in electrolytes [1 M $LiPF_6$/EC-DMC (LP30) and 1 M $LiPF_6$/EC-EMC (Gen 2)] with and without the addition of pyrrole and pyridine were measured by cyclic voltammetry. The results show that the peak current for deintercalation in the cyclic voltammogram is reduced by about 23 percent and 60 percent, suggesting that the additive has an adverse effect on the electrode reaction.

Keywords: Electrolyte Additive, Rechargeable Batteries

164. **DEVELOPMENT OF NON-FLAMMABLE ELECTROLYTES AND THERMAL CHARACTERIZATION**
$90,000
DOE Contact: Ray Sutula (202) 586-8064
Illinois Institute of Technology Contact:
J. Prakash (312) 567-3639

The objective of this program is to develop nonflammable electrolytes with high flash point (>100˚C), ionic conductivity (10^{-3} S/cm), and wider voltage window (0-5 V vs. Li) in an effort to provide better thermal stability and fire safety. A new flame retardant material, hexa-ethoxy-tri-aza-phosphazene ($N_3P_3[OCH_2\ CH_3]_6$), was evaluated by cyclic voltammetry, AC-impedance, and accelerated rate calorimetry in EC-DMC/$LiPF_6$ liquid electrolyte. Initial thermal behavior of the new flame-retardant additive looks promising and the performance of the additive in Li-ion cells will be investigated.

Keywords: Non-Flammable Electrolyte, Rechargeable Batteries

165. **NON-FLAMMABLE ELECTROLYTES**
$90,000
DOE Contact: Ray Sutula (202) 586-8064
Covalent Associates, Inc. Contact: A. B. McEwen
(781) 938-1140

The objective of this program is to develop non-flammable electrolytes for Li-ion batteries that meet the goals for high-power and thermal abuse tolerance for transportation applications. The use of ionic liquid based electrolytes for Li-ion battery systems was demonstrated. This project is completed.

Keywords: Non-Flammable Electrolyte, Rechargeable Batteries

166. **ELECTRODE SURFACE LAYERS**
$280,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
F. R. McLarnon (510) 486-4636

The objective of this project is to establish direct correlations between electrode surface changes, interfacial phenomena, and cell capacity decline. Studies to determine the effects of added sulfur on the surface chemistry and morphology of $LiMn_2O_4$ electrodes were completed. The electrode exposed to S at 160˚C exhibited good electrochemical cyclability, whereas the electrode exposed to S at 260˚C displayed no electrochemical activity.

Keywords: Thin Films, Surface Studies

167. **SYNTHESIS AND CHARACTERIZATION OF ELECTRODES**
$190,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
E. J. Cairns (510) 486-5028

The primary objectives are to directly observe Li in BATT Program cathode materials, characterize the Li atomic and electronic local environment, and determine changes in this environment with cycling; and to synthesize intermetallics that have higher capacities than carbon electrodes and that demonstrate stable capacities during cycling. ^7Li MAS NMR spectra of $Li_xTi_yMn_{1-y}O_4$, $Li_xCu_yMn_{1-y}O_4$ and $LiMPO_4$ samples (M = Fe, Mn, Co, Ni) have been obtained.

Keywords: Intercalation Electrodes, Rechargeable Batteries

168. **EQCM STUDIES OF THE SEI ON CARBON ANODES**
$110,000
DOE Contact: Ray Sutula (202) 586-8064
University of California, Berkeley Contact:
J. W. Evans (510) 642-3807

The objective of this project is to investigate the physical and electrochemical properties of passive film formed on carbonaceous anode using *in situ* electrochemical techniques. An extensive study of the passive layer on carbon anodes and Li de/intercalation in various candidate electrolytes (solvent/salt combinations) using the Electrochemical Quartz Crystal Microbalance (EQCM) and other techniques, especially ellipsometry and cyclic voltammetry is continuing.

Keywords: Surface Layer, Rechargeable Batteries

MATERIALS STRUCTURE AND COMPOSITION

169. **R & D FOR ADVANCED LITHIUM BATTERIES**
$320,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
J. B. Kerr (510) 486-6279

The objectives of this project are to determine by a combination of directed polymer synthesis, theoretical calculations, and transport measurements, the upper limits of conductivity of binary salt and single-ion “dry” polymer electrolytes; and how the polymer architectures and salt structures influence the mechanical strength and processability of the polymer electrolyte membranes. Dendrite growth studies have been completed for several electrolyte systems in symmetrical lithium/lithium cells and in Li/V_6O_{13} cells. The results indicate that electrolyte purity and mechanical strength of the separator appear to be the most critical factors that influence dendrite growth.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolytes

170. **COMPOSITE POLYMER ELECTROLYTES FOR LITHIUM AND LITHIUM-ION BATTERIES**
$90,000
DOE Contact: Ray Sutula (202) 586-8064
North Carolina State University/Michigan State University Contacts: S. A. Khan (919) 515-4519 and G. L. Baker (517) 355-9715

The objectives of this project are to develop solid composite electrolytes (CPEs) that are low-cost, have high conductivities, impart electrode-electrolyte interfacial stability, and yield long cycle life. It was demonstrated that adding fumed silica attenuates lithium dendrite formation. Lithium dendrites formed after passing only 0.34 C/cm^2 in the base-liquid electrolyte without fumed silica; however, the voltage behavior of the CPEs with 10 percent fumed silica (A200 or R805) does not indicate lithium dendrite formation during cycling.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolytes

171. **STRUCTURE AND CHARACTERIZATION OF MATERIALS**
$120,000
DOE Contact: Ray Sutula (202) 586-8064
Brookhaven National Laboratory Contact: J. McBreen (516) 344-4513

The objectives of this project are to elucidate the molecular aspects of battery materials and processes by *in situ* synchrotron X-ray techniques and to provide fundamental information needed to improve the design and performance of advanced rechargeable batteries. The X-ray studies on $LiNi_xMn_{2-x}O_4$ materials (x = 0.1, 0.3 and 0.5) were completed.

Keywords: X-Ray Studies, Electrode Materials

172. **INTERFACIAL AND REACTIVITY STUDIES**
$120,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact: P. N. Ross (510) 486-6226

The objective of this project is to establish direct correlations between electrode surface changes, interfacial phenomena, and cell failure. A cell designed for *in situ* electrochemical experiment for the IR microscope is being built and is near completion. It was demonstrated that the rotating ring disk electrode (RRDE) is useful in detecting both reduction and oxidation species soluble in the electrolyte, which helps in identifying SEI layer formation mechanism.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Surface Layer

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

173. **CELL FABRICATION AND TESTING**
$300,000
DOE Contact: Ray Sutula (202) 586-8064
Lawrence Berkeley National Laboratory Contact: K. A. Striebel (510) 486-4385

The objective of this project is to establish a test vehicle for the evaluation of new materials for high-power and low-cost Li-ion cells. The testing of novel materials in a standard cell with preset protocols will provide the necessary link between the invention of novel battery components and the diagnostic evaluation of failure modes, and will accelerate the development of battery-powered EVs. The power fade and cycle capability of commercially available $LiCoO_2$/graphite cells with gel or liquid electrolyte were studied during the development of testing protocols. All of the cells held more than 80 percent of their original capacity during C/2 100 percent DOD cycling for at least 400 cycles.

Keywords: Li-Ion Batteries, Cell Cycling, Power Fade

174. **MODELING OF LITHIUM/POLYMER ELECTROLYTES**
$70,000
DOE Contact: Ray Sutula (202) 586-8064
Northwestern University Contact: M. A. Ratner (847) 491-5652

The objective of this project is to apply molecular dynamics and Monte Carlo simulation to analyze polymer electrolytes, thus developing a microscopic understanding of their stability, structure and conduction properties. The milestone on electronic structure modeling and this project are completed.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolyte

175. **IMPROVED ELECTROCHEMICAL MODELS**
$240,000
DOE Contact: Ray Sutula (202) 586-8064
University of California, Berkeley Contact: J. Newman (510) 642-4063

The objectives of this project are to report important parameters crucial in the operation of advanced secondary electrochemical power systems; to determine transport and other properties for electrochemical applications; and to improve the performance of electrochemical cells by identifying the controlling phenomena. A continuum-scale numerical model is being developed for transport of Li ions and electrons through an SEI film, in order to understand how mechanisms of transport affect rates of side reactions.

Keywords: Electrochemical Phenomena, Solid-State Cells, Electric Vehicles

176. **FAILURE MECHANISMS IN LI-ION SYSTEMS: DESIGN OF MATERIALS FOR HIGH CONDUCTIVITY AND RESISTANCE TO DELAMINATION**
$65,000
DOE Contact: Ray Sutula (202) 586-8064
University of Michigan Contact: A. M. Sastry (734) 764-3061

The primary objective of these studies is to explain and predict the role of conductive and mechanical failures on reduced performance in the baseline systems, by tightly coupled experimental and simulation studies of microscale transport and mechanics phenomena. Experimental conductivity mapping of electrode materials provided by DOE laboratories, using both two-probe and four-probe conduction experiments, with various tip geometries and spacings, is nearly complete.

Keywords: Modeling, Microstructural Characterization

177. **THERMAL MODELING OF Li BATTERIES**
$30,000
DOE Contact: Ray Sutula (202) 586-8064
University of California, Berkeley Contact: J. W. Evans (510) 642-3807

The objective of this task is to predict the thermal behavior (including stability) and efficiency of Li batteries for use in electric or hybrid vehicles. Heat generation rates have been measured on Li-ion cells (Li-cobalt oxide) at 30 and 45˚C with currents of 25, 50 and 100 mA. The cell is very efficient with heat generation being less than 1 percent of the electrical energy when charged and discharged at low rates (<50 mA).

Keywords: Thermal Phenomena, Rechargeable Batteries, Electric Vehicles

OFFICE OF HEAVY VEHICLE TECHNOLOGIES

HEAVY VEHICLE MATERIALS TECHNOLOGY

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

178. **DESIGN, ANALYSIS AND DEVELOPMENT OF LIGHTWEIGHT FRAMES FOR TRUCK AND BUS APPLICATIONS**
$1,350,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Autokinetics, DaimlerChrysler, Alcoa, Tower Automotive, Auto/Steel Partnership

The objective of this project is to develop concepts for lightweight frames for Class 1 and 2 trucks and buses, develop and implement low-cost manufacturing technologies and validate concepts on full size vehicles. Materials under consideration include aluminum, high strength steels, MMCs and polymer matrix composites.

Keywords: Frames, Manufacturing, Lightweight, Trucks, Buses

179. **DEVELOPMENT OF ADVANCED CASTING TECHNOLOGIES FOR PRODUCTION OF HIGH INTEGRITY TRUCK COMPONENTS**
$1,200,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: ORNL, PNNL, Albany Research Labs
Industry Partners: Freightliner, PACCAR, Alcoa

The objectives of this project are: to develop and integrate the necessary hardware and production procedures to implement advanced casting technologies to a level capable of producing high-integrity parts at rates and volumes necessary for truck and automotive applications; to develop the necessary understanding and technology to cast large structural components for Class 8 truck cabs; and to develop modeling and design capabilities for optimizing steel castings for heavy vehicle applications to reduce weight without sacrificing performance.

Keywords: Aluminum Alloy, Casting, Truck and Automotive

180. **ADVANCED FORMING TECHNOLOGIES FOR LIGHTWEIGHT ALLOYS**
$700,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: LANL, PNNL, INEEL, ORNL

The objective of this project is to evaluate new forming technologies for processing lightweight alloys, to use the new process to achieve improved microstructure, properties, performance and control in the production of components for heavy vehicles.

Keywords: Extrusion, Lightweight Alloys, Forming, Superplastic Forming, Magnesium, Aluminum

181. **DEVELOPMENT OF CARBON MONOLITHS FOR SAFE, LOW PRESSURE ADSORPTION, STORAGE, AND RELEASE OF NATURAL GAS**
$600,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of this project is to develop and test monolithic carbon adsorbant materials for the storage of natural gas in heavy vehicles. The goal is to develop the ability to safely store and release sufficient natural gas at low pressure (<1000psi) to power an urban delivery van for 80 miles.

Keywords: Natural Gas Storage, Carbon Monolith

182. **IMPROVED MATERIALS FOR HEAVY VEHICLE BRAKE AND FRICTION APPLICATIONS**
$400,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Honeywell

The objective of these activities is to investigate the nature of changes on surfaces of materials during braking, develop understanding of the role of friction films in braking, to evaluate advanced materials for heavy vehicle brake application and to develop reliable, cost-effective, laboratory-scale friction tests to select and rank new materials and surface treatments for engine components.

Key words: Brakes, Friction Materials, Friction Films

183. **HIGH CONDUCTIVITY CARBON FOAMS FOR THERMAL MANAGEMENT**
$125,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Caterpillar, Modine, Peterbilt

The objective of this activity is to evaluate the use of conductive carbon foam materials as a highly efficient and lightweight heat exchanger for heavy vehicle cooling needs such as radiators, etc. Focus is on determining basic material properties, defining acceptable operating limits and fabrication of the core structures which can operate in a class 7-8 vehicle.

Keywords: Carbon Foam, Heat Exchanger, Heavy Vehicle

184. **ADVANCED JOINING TECHNOLOGY DEVELOPMENT**
$250,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ANL, ORNL, PNNL

The objective of this project is to develop cost-effective technologies for joining lightweight materials as well as dissimilar materials for use in heavy vehicle structures.

Keywords: Friction Stir Processing, Dissimilar Materials, Joining

185. **DEVELOPMENT OF ADVANCED MATERIALS FOR HEAVY VEHICLE APPLICATIONS**
$1,500,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ANL, NIST, ORNL, PNNL

The objective of this project is to evaluate advanced lightweight materials and processes that can potentially reduce weight or enhance the performance and durability of heavy vehicles. Materials that are being considered include magnesium, titanium, metal matrix composites or carbon fiber-reinforced polymer composites, as well as non-conventional materials.

Key words: Advanced Processes, Advanced Materials, Titanium, Magnesium, MMC

186. **IMPLEMENTATION OF LIGHTWEIGHT MATERIALS IN HEAVY VEHICLE STRUCTURAL APPLICATIONS**
$1,550,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
PNNL Contact: Mark Smith (509) 376- 2874
Laboratory Partners: ORNL, PNNL
Industry Partners: Freightliner, PACCAR, Delphi, Volvo

The objective of this project is to develop cost-effective manufacturing processes and design procedures for carbon fiber reinforced composite materials, alone, or together with lightweight metals, for applications aimed at reducing the mass of Class 8 trucks to improve fuel economy. Research efforts are concentrating on both body and frame members and emphasize the use of high performance fibers embedded into commodity grade resin systems. Component and subsystem mass reductions in excess of 50 percent is the goal of each research effort.

Keywords: Carbon Fiber Reinforced Composites, Structural Components, Polymer Processing, Magnesium

187. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,300,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of these activities is: to provide assessment of various technologies, to conduct workshops to assess technology needs for the trucking industry, to develop multi-year program plans and to provide guidance to program management as to appropriate investments for R&D funding and to fund innovative research with small businesses.

Keywords: Cost, Planning, Workshops, Technical Management, Assessments

HIGH TEMPERATURE MATERIALS LABORATORY

188. **HIGH TEMPERATURE MATERIALS LABORATORY USER PROGRAM**
$5,600,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: Arvid Pasto (865) 574-5123

The HTML (High Temperature Materials Laboratory) is a national user facility, offering opportunities for American industries, universities and other federal agencies to perform in-depth characterization of advanced materials under the auspices of its User Program. Available are electron microscopy for microstructural and microchemical analysis, equipment for measurement of the thermophysical and mechanical properties of materials to elevated temperatures, X-ray and neutron diffraction for structure and residual stress analysis, high speed grinding machines and measurement of component shape, tolerances, surface finish and friction and wear properties.

Keywords: Materials Characterization, Ceramics, Composites, Alloys, Components

OFFICE OF POWER TECHNOLOGIES

	FY 2001
OFFICE OF POWER TECHNOLOGIES - GRAND TOTAL	$73,557,000
OFFICE OF SOLAR ENERGY TECHNOLOGIES	$36,117,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$22,058,000
Amorphous Silicon for Solar Cells and Polycrystalline Thin-Film Materials for Solar Cells	17,381,000
Film Silicon for Solar Cells	1,577,000
Deposition of Solar Grade Silicon	300,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,800,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$12,119,000
Materials and Device Characterization	5,449,000
Materials Structure and Composition	6,670,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,000,000
High-Efficiency Crystalline Silicon Solar Cells	1,300,000
Instrumentation and Facilities	700,000
OFFICE OF WIND AND GEOTHERMAL TECHNOLOGIES	$940,000
Non-Destructive Testing of Corrosion- and Erosion-Induced Damage in Geothermal Piping Systems	275,000
Design Criteria and Structural Response Analysis for Well Cements	165,000
High Performance Polymer Coating Materials	100,000
Field Demonstration and Evaluation of Lined Heat Exchanger	220,000
Acid Resistant Cements	150,000
High-Temperature Polymeric Elastomers	30,000
OFFICE OF HYDROGEN AND SUPERCONDUCTIVITY TECHNOLOGIES	$36,500,000
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS	$36,500,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$36,500,000
The Second Generation Wire Development	12,000,000
The Superconductivity Partnership Initiative	14,000,000
The Strategic Research	10,500,000

OFFICE OF POWER TECHNOLOGIES

OFFICE OF SOLAR ENERGY TECHNOLOGIES

The National Photovoltaics Program sponsors research and development with the goal of making terrestrial solar photovoltaic power a significant and commercially viable part of the national energy mix. From such efforts, private enterprise can choose options for further development and competitive application in U.S. and foreign electric power markets. Approximately 70 percent of the domestic product is exported to developing countries. The objective of materials research is to overcome the technical barriers that limit the efficiency and cost effectiveness of photovoltaic cells. Conversion efficiency of photovoltaic cells is limited by the spectral response of the semiconductor (dependent on band structure), carrier mobility, and device engineering factors. These factors include junction depth, reflection coefficient, parasitic resistances (i.e., series resistance in the metallization and contacts, shunt resistance through the thickness of the cell), and material imperfections that support dark recombination of excess photogenerated carriers. Manufacturing cost is affected by the expense of semiconductor material growth, the complexity of junction formation and cell fabrication, and the material requirements of final module assembly. While most photovoltaics in the U.S. have (historically) been intended for remote standalone applications, an increasing number of domestic deployments are intended for a grid-tied (net metering) environment. World-wide photovoltaic module production in CY 2001 is expected to be approximately 340 MW, with about 90 MW made in the U.S.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

189. **AMORPHOUS SILICON FOR SOLAR CELLS and POLYCRYSTALLINE THIN-FILM MATERIALS FOR SOLAR CELLS**
$17,381,000
DOE Contact: Jeffrey Mazer: (202) 586-2455
NREL Contacts: Bolko von Roedern (303) 384-6480 and Harin Ullal (303) 384-6486

Amorphous Silicon: These projects perform research on the deposition and characterization of amorphous silicon thin films to improve solar cell conversion efficiency and high-throughput manufacturability. Efficient conversion is hindered by unintended impurities or undesired structure in the deposited films and by poor uniformity of the films over large (4000 cm^2) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition, and sputtering. The long term goal is to develop technology for 15 percent efficient (stabilized) photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of amorphous Si-based PV in large-scale distributed power scenarios.

Polycrystalline Thin Films: These projects perform applied research on the deposition of $CuIn(Ga,S)Se_2$ (CIGSS) and CdTe thin films for solar cells. Research is focused on improving conversion efficiency by depositing more nearly stoichiometric CIGSS and CdTe films, by controlling interlayer diffusion and lattice matching in heterojunction structures, and by controlling the uniformity of deposition over large (4000 cm^2) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition, and sputtering. The long term goal is to develop technology for 15 percent efficient photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of polycrystalline film-based PV in large-scale distributed power scenarios.

Keywords: Amorphous Silicon, Amorphous Materials, Polycrystalline Films, Copper Indium Diselenide, Cadmium Telluride, Coatings and Films, Chemical Vapor Deposition, Sputtering, Physical Vapor Deposition, Electrodeposition, Semiconductors, Solar Cells

190. **FILM SILICON FOR SOLAR CELLS**
$1,577,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Ted Ciszek (303) 384-6569 and Harin Ullal (303) 384-6486

These projects perform applied research on the high-throughput deposition of relatively thin crystalline silicon (50-100 microns). Methods include recrystallization of silicon powder on inexpensive ceramic substrates, and are amenable to rapid thermal annealing (RTA) and integrated module manufacturing techniques. The goal is to develop highly cost effective crystalline silicon modules, with conversion efficiencies in the 12-14 percent range.

Keywords: Crystalline Silicon, Film Silicon, Recrystallization, Rapid Thermal Annealing, Semiconductors, Solar Cells

191. **DEPOSITION OF SOLAR GRADE SILICON**
$300,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Ed Witt (303) 384-6402 and
Ted Ciszek (303) 384-6569

This project has the goal of achieving a low-cost (~$15/kilogram) crystalline silicon feed stock material suitable for commercial solar cell production. The method involves the refining of liquid metallurgical grade silicon. Such material could prove critical to photovoltaic commercial expansion in the event that large quantities of reject electronic-grade silicon feed stock from the integrated circuit industry become unavailable.

Keywords: Solar Grade Silicon, Metallurigical Grade Silicon, Solar Cells, Crystalline Silicon Solar Cells, Crystalline Silicon

192. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$2,800,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Sarah Kurtz (303) 384-6475 and
Robert McConnell (303) 384-6419

These projects perform research on the deposition and conduction properties of III-V semiconductors for super high efficiency concentrator solar cells. Research is focused on precise deposition of layers, elucidation of the properties of the interfacial regions, and improved understanding of the conduction limiting mechanisms of the materials. Conduction limiting mechanisms are particularly severe in the case of GaInAsN, an otherwise almost ideal material for use in a four-junction super high efficiency concentrator cell. The materials are deposited by metal organic chemical vapor deposition, liquid phase epitaxy, and molecular beam epitaxy. The long-term goal is to develop three- and four-junction III-V-based cells that achieve as much as 40 percent efficiency under high-ratio concentration.

Keywords: Gallium Arsenide, III-V Materials, High-Efficiency Solar Cells, MOCVD, MBE, Liquid-Phase Epitaxy, Quaternary Semiconductors, Semiconductors, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

193. **MATERIALS AND DEVICE CHARACTERIZATION**
$5,449,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Pete Sheldon (303)384-6533

These projects measure and characterize material and device properties. Approaches include surface and interface analysis, electro-optical characterization, and cell performance and material evaluation. These allow study of critical material/cell parameters such as impurities, layer mismatch, and other defects that limit photovoltaic performance and lifetime. Specific techniques include deep level transient spectroscopy, electron beam induced current, secondary ion mass spectroscopy, scanning electron microscopy and scanning transmission electron microscopy, Auger spectroscopy, Fourier-transform based measurements (e.g., FT-Raman, FTIR, and FT-PL), radio-frequency photoconductive decay, ellipsometry, and photoluminescence.

Keywords: Nondestructive Evaluation, Surface Analysis, Surface Characterization, Semiconductor Microstructure, Analytical Microscopy, Charge Carrier Lifetime Measurement, Semiconductor Defects, Solar Cell Testing, Module Testing

194. **MATERIALS STRUCTURE AND COMPOSITION**
$6,670,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Alex Zunger (303) 384-6672 and
Robert McConnell (303) 384-6419

These projects support the fundamental and exploratory research needed for advancement of PV technologies in the long term—five to ten years—and beyond. Projects include collaboration with Office of Science (SC). Topics include ordering in ternary and quaternary materials, solid state spectroscopy, solid state theory of photovoltaic semiconductors, computational material sciences, structure of photoelectrochemical materials such as dye-sensitized solar cell materials, properties of transparent conducting oxides, structure of GaInAsN alloys, impurity precipitation and dissolution in crystalline silicon, and structure of hydrogen incorporation in silicon materials.

Keywords: Semiconductor Structure, Solid State Spectroscopy, Ordering in Semiconductors, Photoelectrochemical Materials, Semiconductor Defects, Crystalline Defects, Semiconductor Impurities, Quaternary Semiconductors

DEVICE OR COMPONENT FABRICATION, BEHAVIOR

OR TESTING

195. **HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS**
$1,300,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: John Benner (303) 384-6496, Ted Ciszek (303) 384-6569 and Richard Mitchell (303) 384-6479

This project performs applied research on crystalline silicon materials and devices to improve conversion efficiency in a commercially-compatible process. Methods employ advanced back-surface fields and silicon nitride and other bulk passivation treatments to reduce minority carrier recombination at cell surfaces and in the bulk. Control of point defects in crystalline silicon is studied by a variety of techniques, and is thoroughly discussed at the NREL-sponsored Silicon Devices and Materials Conference held in Colorado each August. Much work is done at the DOE Center of Excellence in Photovoltaics at Georgia Institute of Technology. One of the major goals of this project is to develop a rapid-thermal-processing (RTP)-based, screen-printed-contact, photolithography-free protocol that will yield 18 percent efficient 100 cm^2 cells on crystalline material. Two promising materials for achieving this goal are multicrystalline silicon made by the Heat Exchange Method (HEM) and single-crystal silicon made by the Tri-Crystal Czochralski growth method. In particular, tri-crystals allow for thinly-sawed wafers (~150 to 200 microns) and, when used with excellent surface texturing and an efficient back-surface field, will likely yield a very efficient silicon solar cell in a commercially-compatible process.

Keywords: Crystalline Silicon, Multicrystalline Silicon, High-Efficiency Silicon Cell, Screen Printing Metallization, Light Trapping, Back-Surface Field, Rapid Thermal Processing, Crystalline Silicon Defects, Point Defects, Hydrogen Passivation, Silicon Nitride Passivation, Tri-Crystals, Heat Exchange Method (HEM)

196. **INSTRUMENTATION AND FACILITIES**
$700,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Larry Kazmerski (303) 384-6600

This project procures modern in-house equipment at NREL, primarily for the measurement and characterization of photovoltaic semiconductor materials. This includes equipment for such measurements as ellipsometry, Auger analysis, current-voltage characteristic, Fourier transform-based spectroscopy, electron microscopy; and also includes equipment such as MBE, ECR plasma, and sputtering systems for the fabrication of photovoltaic and related materials.

Keywords: Semiconductor Measurement Equipment, Semiconductor Material Measurement, Semiconductor Characterization, Fourier Transform Spectroscopy, Solar Cells

OFFICE OF WIND AND GEOTHERMAL TECHNOLOGIES

The primary goal of the geothermal materials program is to ensure that the private sector development of geothermal energy resources is not constrained by the availability of technologically and economically viable materials of construction. This requires the performance of intermediate and long-term high-risk materials R & D.

197. **NON-DESTRUCTIVE TESTING OF CORROSION- AND EROSION-INDUCED DAMAGE IN GEOTHERMAL PIPING SYSTEMS**
$275,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M. L. Berndt (631) 344-3060 and A. J. Philippacopoulos (631) 344-6090

This project addresses the need for improved instrumentation and non-destructive testing (NDT) to detect corrosion and erosion-corrosion of geothermal piping systems. Emphasis is placed on evaluating the suitability of certain long-range NDT methods for on-line inspection. Such methods have the ability to locate damage a significant distance from a single sensor and offer reduced inspection costs and improved probability of detection. It is also possible to use these methods for continuous monitoring of pipe condition. Long-range ultrasonic guided waves and dynamic response testing are under investigation. Numerical modeling necessary to establish parameters and to develop an understanding of the nature of the response obtained in these methods is integrated with experimental studies. Samples of piping removed from geothermal plants are used to model the typical types of damage encountered. The project also investigates integration of NDT results with remaining strength and life assessment. The benefits of this work will be improved methodologies for condition assessment and subsequent increase in plant reliability and reduction of maintenance costs.

Keywords: Geothermal Piping, Non-Destructive Testing, Corrosion, Plant Reliability, Ultrasonics, Guided Waves

198. **DESIGN CRITERIA AND STRUCTURAL RESPONSE ANALYSIS FOR WELL CEMENTS**
$165,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M. L. Berndt (631) 344-3060 and A. J. Philippacopoulos (631) 344- 6090

The current design criteria specified for geothermal well cements oversimplify the mechanical property requirements. Minimum unconfined compressive strength at 24 hours is typically specified yet the response to *in situ* loads and ultimate performance rely on additional properties such as elastic modulus, strength under tensile and multi loading scenarios, and the time- and temperature-dependent nature of these properties. Studies are performed to develop an understanding of the nature of the stress regime in the vicinity of geothermal wells. Systematic modeling of the geothermal well behavior is carried out in order to evaluate how cements actually behave *in situ*. For application to well casing remediation, the interactions of system components in remediated wells were analyzed along with development and property description of special cements required for patching. Geomechanical and structural models were developed to evaluate global and local response to axial and shear deformation. Modeling requires comprehensive definition of material properties in the range of the deformations experienced by geothermal wells and prediction of *in situ* behavior so that optimal well life is achieved. Such properties are evaluated through a detailed experimental material characterization program that is carried interactively with modeling studies.

Keywords: Geothermal Wells, Casing Remediation, Cements, Material Testing, High-Temperature Properties, Structural Analysis

199. **HIGH PERFORMANCE POLYMER COATING MATERIALS**
$100,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contact Toshifumi Sugama (631) 344-4029

This project is for the development of organic, inorganic, and organometallic polymer coating systems to mitigate corrosion, oxidation, and abrasive wear in tubing, heat exchangers, piping, vent gas blowers, cooling condensers, and plant structural components made from different metals. Using semi-crystalline high-temperature performance polyaryl and polyfluorocarbon polymers as the matrix for these coatings, the key issue in designing the coating systems to meet the material criteria was to improve their surface hardness and their toughness. To achieve this goal, two different additives, organic or inorganic fibers, and hydraulic or non- hydraulic ceramic fillers, were incorporated into the polymers. The test panels coated with the additive-reinforced polymer composites are being evaluated in an autoclave containing brine at temperatures up to 200˚C. Once potential composite coating systems are identified, large-sized metal panels coated with these systems will be send to geothermal power plants for long-term performance tests.

Keywords: Coating, Polymer Composite, Ceramic Filler, Anti-Corrosion, Abrasive Wear Resistance

200. **FIELD DEMONSTRATION AND EVALUATION OF LINED HEAT EXCHANGER**
$220,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is to optimize the formulation of polyphenylenesulfide (PPS)-based material systems possessing excellent thermal conductivity and corrosion/fouling resistance for use as lining materials for inexpensive carbon steel-heat exchanger tubes and sheets. Tubes lined with PPS material systems are being exposed for extended periods at geothermal power plant site. To date, a year long field test showed that the anti-oxidant PPS liner displayed an outstanding performance in protecting the tube against corrosion caused by 160˚C brine and also fouling by scale deposits. The task also includes installing a state-of-the-art lining apparatus that allows us to fabricate and repair the liners in the field. The post-approval tests for this apparatus are being undertaken to determine its technical feasibility, as well as to verify the reproducibility of the liners deposited on the 40-ft.-long tubes.

Keywords: Polyphenylenesulfide, Thermal Conductivity, Heat Exchanger Tube, Anti-Corrosion, Liner

201. **ACID RESISTANT CEMENTS**
$150,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is designed to develop acid-resistant, tough, resilient calcium aluminate polyphosphate (CaP) composite cementitious materials for supporting and protecting metallic casing pipes against corrosion in CO_2-rich geothermal wells at brine temperatures up to 300˚C and a pH of 1.8. To obtain such desirable properties, a CaP cement was modified with silicon- and fluorine-based chemicals as anti-acid admixtures, and reinforced with carbon and ceramic fibers. The modified and reinforced CaP cement composites are being exposed in autoclave tests to validate that these admixtures and fibers adequately abate acid-erosion and sufficiently increase ductility. The formulation of, and technology for, making these cement composites will be transferred to the geothermal drilling and cementing industry who will evaluate their full-scale technical and economical feasibility.

Keywords: Calcium Aluminate Polyphosphate Cement, Acid-Resistance, Casing Pipe, Fiber Reinforcement, Anti-Acid Admixture

202. **HIGH-TEMPERATURE POLYMERIC ELASTOMERS**
$30,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

The objective of this task is to identify potential elastomeric materials for use in bearing systems in down-hole pumps. The pumps extract the energy resource from geothermal brine reservoirs at 150˚C. Elastomeric bearings made of three candidate polymers, polynitril, polyfluorocarbon, and ethylene-propylene-diene terpolymer (EPDM), were exposed for six months in reservoirs. Hydrothermal oxidation was the major factor affecting the degradation of elastomers. We recommended the oxidation tracing of the profile of exposed bearings as the most effective method for predicting their useful lifetime. Among polymers, EPDM had the lowest degree of oxidation. A long-term exposure test of an EPDM bearing is being undertaken to ensure that it has a useful lifetime of at least 10 years.

Keywords: Bearing Elastomers, Hydrothermal Oxidation, Down-hole Pumps, EPDM

OFFICE OF HYDROGEN AND SUPERCONDUCTIVITY TECHNOLOGIES

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

The DOE Superconductivity Program for Electric Systems works in partnership with industry to perform the research and development required for U.S. companies to commercialize High Temperature Superconductivity (HTS) for electric power applications. To achieve commercialization of the technology, the Superconductivity Program engages in research and development which aims to 1) improve the performance of superconducting wire while reducing manufacturing costs (Wire Technology), 2) demonstrate the applicability and the potential benefits of superconductivity in electric power systems (Systems Technology), and 3) conduct the fundamental investigations necessary to support the wire and systems development (Strategic Research).

Wire research seeks methods to produce HTS wire that has higher current carrying capacity, better magnetic field capabilities, reduced manufacturing costs, and better application characteristics such as durability, flexibility, and tensile strength. Near-term research in this area focuses on conquering scale-up issues of mass-production wire technologies for coated conductor YBCO (yttrium barium copper oxide). Longer-term wire research activities are investigating TBCCO (thallium barium calcium copper oxide) and other compounds for coated conductors, as well as the investigation of underlying superconductivity physics.

Systems research and development activities focus on the research, development, and testing of prototype HTS power system applications through industry-led projects. Research teams investigate adaptability issues for using superconducting wire in power system applications, which include transmission cables, generators, transformers, fault-current limiters, and flywheel electricity systems. In addition, program efforts target end-user applications in energy-intensive industries, including large electric motors (over 5,000 HP), MRI medical units, and magnetic separators. Application issues include the development of efficient cryogenic systems, cable winding techniques, and magnetic field research.

Strategic research conducts advanced, cost-shared, fundamental research activities to better understand relationships between the microstructure of HTS materials and their ability to carry large electric currents over long lengths. New projects will be added to investigate the varied technical aspects of this key problem. The benefit will be higher performance wires and inherently lower manufacturing costs. Also, work on enabling technologies such as joining HTS conductors to normal conductors will be supported as well as additional research on electrical losses due to alternating currents. These losses can be reduced through better understanding of technical parameters. This research will support new discoveries and innovations for the Second Generation Wire Development. These efforts complement research work funded by the DOE Office of Science. This subprogram includes work on planning and analysis of potential program benefits as well as communication and outreach to gather information on future requirements for the HTS technologies and to maintain contact with stakeholders.

203. **THE SECOND GENERATION WIRE DEVELOPMENT**
$12,000,000
DOE Contact: Jim Daley (202) 586-1165
Industry Partners: American Superconductor
Contact: Gilbert N. Riley (508) 836-4200
Intermagnetics General Corp. Contact:
Roger Farrell (518) 346-1414
Oxford Superconducting Technology Contact:
Seung Hong (732) 541-1300
3M Contact: Arnold Funkenbusch (651) 733-5071
MicroCoating Technologies Contact:
Shara Shoup (678) 287-2478

National Laboratories: Argonne National
Laboratory Contact: U. Balachandran
(630) 252-4250
Brookhaven National Laboratory Contact:
David Welch (516) 282-3517
Los Alamos National Laboratory Contact:
Dean Peterson (505) 665-3030
National Renewable Energy Laboratory Contact:
Richard Blaugher (303) 384-6518
Oak Ridge National Laboratory Contact:
Robert Hawsey (615) 574-8057
Sandia National Laboratory Contact:
Jim Voigt (505) 845-9044

The Second Generation Wire Development capitalizes on two processing breakthroughs announced in 1995 and 1996: the Ion-Beam Assisted Deposition (IBAD) process refined by LANL and the Rolling Assisted Biaxial Texturing (RABiTS) technique pioneered by ORNL. Since then, industry-led consortia have evolved to develop these techniques into viable commercial processes for making HTS wire. In FY 2001, Los Alamos and Oak Ridge National Laboratories were provided with cutting-edge facilities and instrumentation to establish "Research Park" environments where industry researchers can be stationed for extended periods to work with national laboratory scientists in accelerating the development, commercialization, and application of second-generation, high temperature superconductor wires.

Project subtasks are as follows:

Metallo-Organic Chemical Vapor Deposition (MOCVD) - Investigation continued on the development of a MOCVD technique for deposition of long-length, Yttrium-Barium-Copper Oxide (YBCO) conductors. The goal is to establish processing conditions to deposit buffer and superconducting layers on textured metallic substrates. The substrates, buffer, and superconducting layers will be characterized.

Thick HTS Films - Teams made significant progress in 2001 in the development of thick HTS films. The films will be deposited on flexible tapes containing oxide buffer layers deposited by IBAD. Efforts included analysis of electrical flow in thick films, and the development of new diagnostic techniques for identifying "bottlenecks" in the superconductors.

Substrate Development - Efforts at producing long lengths of textured nickel tape with all the appropriate characteristics for subsequent film growth (buffer layer(s) and superconductor) were continued. Work on a two-year project with the goal of producing 1-meter lengths of buffered, textured nickel (RABiTS) and YBCO on RABiTS with a target critical current density (J_c) of 80,000 A/cm^2 also continued.

IBAD Research - Program partners were completing the first phase of research on the IBAD approach. Electron beam evaporation is 3M's selected method of deposition of all the layers. ORNL worked to characterize bare, textured nickel and films grown by a variety of techniques, and to develop buffer layer and superconductor deposition technology. ORNL continued pursuing a promising alternative to *in situ* formation of the YBCO film, by electron beam co-evaporation of Y, Ba, and Cu. ORNL scientists worked on determining the thickness limits of epitaxial film formation, and assessing the feasibility of rapid precursor depositions for the *ex situ* precursor reaction process.

YBCO/RABiTS - Development and demonstration of the fabrication of lengths of YBCO/RABiTS using MOCVD technology continued. Mechanical and processing conditions needed to develop the desired surface texture and smoothness of the bare nickel were investigated. In addition to providing samples of short and long-length RABiTS, program researchers continued to characterize products for uniformity of texture and electrical and mechanical properties.

Keywords: Superconductor, Coated Conductor, Buffer Layers, Deposition, Textured Substrate

204. **THE SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE**
$14,000,000
DOE Contact: Jim Daley (202) 586-1165

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy (DOE) and industrial consortia intended to accelerate the use of high-temperature superconductivity (HTS) in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the research and development (R&D) cycle. That is, the teams include the ultimate user of the technology (an electric power company), as well as a major manufacturing company, and a supplier of superconducting components. Each team also includes one or more national laboratories that perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery, and use. The funding provides DOE's 50 percent cost share of the SPI design activities, prototype development, and operational testing. All of these projects incorporate high-temperature superconducting wire into an electric power application.

Project subtasks are as follows:

Fault-Current Controller - LANL Researchers continued efforts to optimize the performance of a demonstration HTS Current Controller developed by General Atomics. Current controllers can be used on transmission and distribution systems to protect system components from damaging power surges caused by ground faults. Compared to conventional devices, HTS current controllers offer better protection and improved system flexibility, reliability, and performance. The testing was completed and the unit has been relocated to Los Alamos National Laboratory (LANL) for tests designed to optimize its performance.

LANL Contact: Dean Peterson (505) 665-3030

HTS 1,000 hp and 5,000 hp Motors - The project, led by Rockwell Automation, completed operational testing of a 1,000 horsepower (hp) motor in 2001. Rockwell's Reliance Electric division assembled the motor, which incorporates HTS coils fabricated and wound by American Superconductor. Design analysis and preliminary system component testing for a 5,000 hp unit was completed. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. These reduced losses and the smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.

Rockwell Automation Contact: David Driscoll
(216) 266-6002

Cold Dielectric Superconducting Transmission Cable - Southwire Company and Oak Ridge National Laboratory (ORNL) continued a partnership centered on the development of a power cable for real-world applications. The 30-meter, three-phase HTS cable feeding electricity to three Southwire manufacturing facilities surpassed 10,000 hours of continuous operation in 2001, and operated in an unsupervised environment for most of the year. Other efforts concentrated cable termination designs, bending analyses, and splices.

Southwire Contact: R. L. Hughey (770) 832-4984

Warm Dielectric Superconducting Transmission Cable - A team led by Pirelli Cables and Systems and including Detroit Edison, American Superconductor, and Los Alamos National Lab installed a 120-meter, 3-phase, room-temperature dielectric HTS power cable system in a Detroit Edison substation. Cable operational testing is beginning in 2001. The HTS cable will lead to more efficient electricity transmission lines in utility networks.

Pirelli Contact: Nathan Kelley (803) 356-7762

HTS Flywheel Electricity System - This project involves the development and demonstration of a 10 kWh Flywheel Electricity System. High Temperature Superconducting bearings (single crystal YBCO superconductor material) are an enabling technology for the flywheel design. The bearings allow the flywheel to store electricity with increased efficiency. Scientists at Boeing and Argonne National Laboratory completed the component testing and assembly of the device in 2001. The system has performed well in operational tests and will lead to the demonstration of a second unit, optimized for backup power applications.

Boeing Contact: Mike Strasik (425) 237-7176

Reciprocating HTS Magnetic Separator - This project teams DuPont with the National High-Magnetic Field Laboratory to develop a reciprocating magnetic separator. These devices are used in mineral extraction and purification and are traditionally large consumers of electricity. In 2001, a demonstration unit was assembled and tested. The unit exceeded expectations, and DuPont is moving toward developing a pre-commercial unit in 2002.

DuPont Contact: Chris Rey (302) 695-9470

HTS Transformer - Waukesha Electric Systems (WES) is leading a team that includes ORNL, IGC-SuperPower, and Rochester Gas and Electric to build and operate a 5/10 MVA prototype cryogenically-cooled HTS power transformer for testing on the Wisconsin Electric Power grid. The prototype will power WES' main transformer manufacturing plant. In 2001, the team began assembling the components of the device, and site preparation was completed.

Waukesha Contact: Sam Mehta (262) 547-0121

Keywords: Motor, Current Controller, Transmission Cable, Flywheel, Separator

At the end of August 2001, the High Temperature Superconductivity (HTS) Program selected seven proposals for negotiation of new SPI Cooperative Agreements. The selected proposals and the Team Leaders are: "Superconducting Flywheel Power Risk Management System" submitted by Boeing Phantom Works (Seattle, WA); "Demonstration of a Pre-Commercial Long-Length HTS Cable System Operating in the Power Transmission Network" submitted by Pirelli Cables & Systems (Lexington, SC); "Design and Development of a 100 MVA HTS Generator" submitted by General Electric Corporate Research and Development (Niskayuna, NY); "Pre-Production High Temperature Superconducting Reciprocating Magnetic Separator" submitted by DuPont Company (Wilmington, DE); "Long Length High Temperature Superconducting Power Cable" was submitted by a team led by Southwire Company (Carrollton, GA); "Cost Effective, Open Geometry HTS Magnetic Resonance Imaging System" was submitted by a team led by Oxford Instruments (Carteret, NJ); and "Transformer Component, High Temperature

Superconducting Substation" submitted by IGC-SuperPower (Schenectady, NY).

205. **THE STRATEGIC RESEARCH**
$10,500,000
DOE Contact: Jim Daley (202) 586-1165

Strategic research and development projects in the program are crucial for the discovery of new technologies, such as RABiTS and magneto-optical imaging (MOI), that make the program a world leader in the race to bring HTS electric power technologies to market. Critical theoretical calculations, new material evaluation, and process development support the program's industry-directed Cooperative Research and Development Agreement (CRADA) work and the SPI application projects and provide a foundation for future collaborations and progress toward HTS commercialization by industry.

Work by all organizations in strategic research comprises a diverse set of topics from characterization techniques to wire processing to applications development. As these activities mature, they evolve into more cohesive efforts devoted to improving mechanical and electrical properties of wire and new devices.

Project subtasks are as follows:

Strategic projects continued to focus on the development of improved substrates for both IBAD and RABiTS processes, and deposition processes for buffer layers and the superconductor layer. Characterization of buffer and superconductor layers attempted to correlate processing parameters with final wire performance. Projects were active at all six national laboratories.

University Collaborations - Argonne National Lab continued to operate five active university collaborations: 1) Development of dielectric substrates for coated conductors (with Pennsylvania State University); 2) Development of stable MOCVD precursors for buffer and YBCO layers (with Northwestern University); 3) Pulsed laser deposition of YBCO on textured substrates (with Iowa State University); 4) Understanding the fundamentals of film growth in the MOCVD process (with the University of Illinois at Chicago); and 5) Kinetics of YBCO crystallization from melts (with the University of Houston).

Wire Characterization - Program participants were completing the characterization of microstructural and superconducting properties of second-generation wire to improve understanding of J_c-limiting factors related to the formation and growth kinetics of high-temperature superconductors. On-line characterization instruments are being developed to maintain quality control in the fabrication of long lengths of HTS wire. The engineering scale-up will require the integration of characterization and the process control of the fabrication parameters.

Oxide Buffer Layer Research - Work on developing sol-gel derived oxide buffer layer systems continued in 2000. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

Coated Conductor Processing - Research and development of YBCO and Thallium-Barium-Calcium-Copper Oxide (TBCCO) coated conductor processing continued in a variety of subtasks. Scale-up issues are being defined and addressed. Developing the capability to fabricate 1- to 2-m lengths of RABiTS, using electron beam evaporation and an existing ultra-high vacuum, reel-to-reel system remained a priority. Lengths of RABiTS were being provided for internal use as well as for various partners.

PLD Deposition - A system and process for deposition of YBCO by Pulse Laser Deposition on moving substrates was being developed by the utilization of a radiant heating system, along with sample translation. Also, improved texture in substrates with reduced magnetism was under development. Deposition studies of TBCCO on RABiTS continued, and new RABiTS architectures, with conductive and simpler structures, were investigated.

Process Technology - DOE partners worked toward developing and demonstrating process technology needed for epitaxial growth of buffer layers by metalorganic decomposition. A specific objective of the project is to develop alkoxide precursor methods for deposition of buffer layers compatible with textured metallic substrates appropriate to long-length conductor manufacture and compatible with American Superconductor's YBCO deposition methods.

The program supports a broad range of activities which concentrate on the underlying principles of HTS and developing an understanding of how these principles affect final HTS material properties. Collaborators in the activities have worked on understanding reaction kinetics, effects of stoichiometry on the superconducting properties, introducing flux pinning centers, and monitoring current transport in HTS conductors.

ORNL funded three university research and development projects in FY 2001. Researchers at Stanford University investigated ion-beam assisted deposition of buffer layers and *in situ* deposition of YBCO by electron beam evaporation. The University of Wisconsin conducted research on BSCCO critical currents and microstructures, YBCO coated conductor microstructure, and pulse tube cryocooler technology. Finally, researchers at the

University of Houston continued investigation of high-rate photon-assisted metallo-organic chemical vapor deposition for YBCO onto buffered, textured metallic substrates.

<u>AC Loss Characterization</u> - Attempts to characterize AC losses in HTS tapes, under conditions which simulate the electromagnetic conditions in utility devices, continued. Program participants worked to design a cable configured to minimize AC losses.

Keywords: Superconducting Tapes, Flux Pinning, Thallium Conductor, Bismuth Conductor

OFFICE OF SCIENCE

	FY 2001
OFFICE OF SCIENCE - GRAND TOTAL	$551,082,034
OFFICE OF BASIC ENERGY SCIENCES	$501,008,000
DIVISION OF MATERIAL SCIENCES AND ENGINEERING	$501,008,000
Theoretical Condensed Matter Physics	16,124,000
Experimental Condensed Matter Physics	35,837,000
Materials Chemistry	30,808,000
Mechanical Behavior and Radiation Effects	15,286,000
Neutron and X-ray Scattering	31,682,000
Structure and Composition of Materials	33,767,000
Physical Behavior	16,449,000
Synthesis and Processing Sciences	12,801,000
Engineering Research	17,352,000
Experimental Program to Stimulate Competitive Research	7,685,000
National User Facilities (Materials Research)	283,217,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$41,474,034
DIVISION OF TECHNOLOGY RESEARCH	$41,474,034
LABORATORY TECHNOLOGY RESEARCH PROGRAM	$3,980,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING	$2,578,000
Advanced Processing Techniques for Tailored Nanostructures in Rare-Earth Permanent Magnets (AL 01 02)	40,000
Improved Materials for Semiconductor Devices (PNL 98 17)	117,000
Development of High-Temperature Superconducting Wire Using RABiTS Coated Technologies (ORNL 97 02)	30,000
Development of Bismuth-Based Superconducting Wire With Improved Current Carrying and Flux Pinning Properties (ANL 99 15)	300,000
Light Emission Processes and Dopants in Solid State Light Light Sources (LBNL 97 13)	11,000
Development of Buffer Layers Suitable for Deposition of Thick Superconducting YBCO Layers by a Post-Deposition Annealing Process (BNL 98 05)	125,000
Interplay Between Interfacial and Dielectric and Ferroelectric Behaviors of Barium Strontium Titanate Thin Films (PNL 99 08)	278,000
Efficiency Improvement of Nitride-Based Solid State Light-Emitting Materials (LBNL 01 04)	20,000
Advanced Computatioal Models and Experiments for Deformation of Aluminum Alloys – Prospects for Design (PNL 99 07)	278,000
Near-Frictionless Carbon Coatings (ANL 98 03)	300,000
Fundamental Scientific Problems in Magnetic Recording (ORNL 01 04)	40,000
Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface (LBNL 98 10)	189,000
An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry (LBNL 98 16)	210,000
Interfacial Properties of Electron Beam Cured Composites (ORNL 99 08)	300,000
Photocatalytic Metal Deposition for Nanolithography (ANL 99 13)	300,000
Low-Cost, High-Performance YBCO Conductors (ORNL 01 06)	40,000

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
LABORATORY TECHNOLOGY RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,402,000
Nanofabrication of Advanced Diamond Tools (LBNL 01 03)	34,000
Ionically Conductive Membranes for Oxygen Separation (LBNL 97 03)	35,000
Alloy Design and Development of Cast Cr-W-V Ferritic Steels for Improved High-Temperature Strength for Power Generation Applications (ORNL 01 08)	33,000
Highly Dispersed Solid Acid Catalysts on Mesoporous Silica (PNL 97 28)	48,000
Development of a High-Efficiency Rotary Magnetocaloric Refrigerator Prototype (AL 99 02)	300,000
Direct Casting of Titanium Alloy Wire for Low-Cost Aerospace and Automotive Fasteners (PNL 99 02)	278,000
Nonconsumable Metal Anodes for Primary Magnesium Production (ANL 98 05)	300,000
Development of Electrolyte and Electrode Materials for Rechargeable Lithium Batteries (BNL 98 04)	74,000
Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks (LBNL 99 01)	300,000
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$36,244,071
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$19,587,989
PHASE I	$3,298,130
Fabrication of Polyimide Inertial Fusion Energy Target Capsules by a Fully Automated Process	99,894
Sealed, High-Heat Capacity, Cable-in-Conduit Superconductors	100,000
A Novel Reactive Processing Method to Join SiC Components for Fusion Applications	100,000
Joining of Advanced SiCf/SiCm Composites for Fusion Energy Applications	100,000
A High-Power, Ceramic, RF Generator and Extractor	100,000
Quasi-Optical Millimeter-Wave Accelerating Structure	100,000
KA-Band RF Transmission Line Components for a High-Gradient Linear Accelerator	100,000
A Novel Process for Producing Low Cost Sn-Ti Core Rods for Internal Tin Nb3Sn	99,989
A Scalable APC Process with a Novel Pin Structure for High Field Magnets	100,000
Enabling Technologies for Inline Heat Treatment of Nb3Sn Precursor Cables Suited to Fabrication of Nb_3Sn Flexible Cables	100,000
A Method to Increase Current Density in a Mono Element Internal Tin Process Superconductor Utilizing ZrO_2 to Refine the Grain Size	99,584
Hermetic Metallization of Aluminum Nitride for Radio Frequency Devices	99,984
Detector Arrays Based on Fast Scintillators	99,999
Thick Silicon Photodiodes for High Efficiency X- and Gamma-Ray Spectroscopy	100,000
High Density CZT Array Assembly Techniques	100,000
Truss-Integrated Thermoformed Ductwork	100,000
Reactive Separation via a Hydrothermally Stable Hydrogen Selective Membrane	100,000
Novel Membrane Reactor for the Desulfurization of Transportation Fuels	100,000
Low-Cost Ceramic Modules Incorporating Palladium-Based Membranes for Dehydrogenation Reactions	100,000
Low Emission Diesel Engines	100,000
Selective Adsorption Membranes for the Production of Enriched Air	98,699

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
PHASE I (continued)	
Treatment of Produced Water with Fouling-Resistant Nanofiltration Membranes	100,000
Low-Cost, Large-Membrane-Area Modules for Gas Separation	100,000
An Acoustically Enhanced Pervaporation Bioreactor (APB)	100,000
Novel Thin-Film Ceria Membrane Materials for Small-Scale Oxygen Generation Systems	100,000
Pyrolitic Boron Nitride Neutron Sensitive Direct Converter Layers	100,000
Novel Nanocomposite Anodes for Lithium-Ion Batteries	100,000
Novel Nano-Structured Catalyst for Steam Gasification of Carbonaceous Feedstocks	100,000
Treated Silicate Sorbents for Mercury Removal from Flue Gas	99,994
Control of Catalyst Poisons from Coal Gasifiers	100,000
High-Temperature Highly-Efficient Ceramic Heat Exchanger	99,987
Integrated Membrane System for Upgrading Nitrogen-Rich Natual Gas	100,000
Zero-Emission Natural Gas Glycol Dehydrator System with Improved Drying Capacity	100,000
PHASE II (FIRST YEAR)	$8,459,941
Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating	375,000
Advanced Geothermal Optical Transducer (AGOT)	325,879
Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape	374,999
Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors	300,000
Affinity Ceramic Membranes with Carbon Dioxide Transport Channel	300,095
Photocatalytic Membranes for Producing Ultrapure Water	300,000
Novel Membrane Reactor for Fischer-Tropsch Synthesis	300,000
Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron Emission Tomography Imaging	340,000
Miniature Electrochemical Carbon Dioxide Detector	338,128
An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis	340,000
Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys	375,000
A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells	325,000
Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications	375,000
Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells	350,000
Efficient Incandescent Lighting Based on Selective Thermal Emitters	350,000
‘On Chip’ Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications	350,000
Infrared Focal Plane Array with Fast Shuttering	375,000
Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single Photon Sensitivity	375,000
Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy	374,285

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
PHASE II (FIRST YEAR) (continued)	
Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors	366,561
Micromachined Silicon, Large Area X-Ray Detector	374,994
Cost-Reduction Techniques for Powder-in-Tube Niobium-Tin Superconductors	300,000
Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets	250,000
Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout	375,000
Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal ThermaltoElectric Converters	250,000
PHASE II (SECOND YEAR)	$7,504,950
High-Temperature Oscillator and Digital Clock	373,618
Capacitors for Extreme Temperature Applications	375,000
A High Temperature MEMS Inclination Sensor for Geothermal Drilling	374,612
High Efficiency Thermoelectric Power Conversion Devices	375,000
Fast Repetitive Arc Free Current Limiting Circuit Breaker	374,894
A High Current Very Low Cost $Niobium_3$Tin Titanium Doped Conductor Utilizing a Novel Internal Tin Process, with Separate Stabilizing Elements Scalable to Modern Niobium Titanium Production Economics	300,000
Automated Diamond Turning Lathe for the Production of Copper Accelerator Cells	375,000
High Power Switch	313,798
Adiabatic Forming of Copper Accelerator Cells for the NLC	375,000
Low Cost Support Structures, With New Advanced Composite Materials Tailored for Ultra-Stable Particle Tracking Detectors	337,031
SQUID Susceptometers for Read Out of Magnetic Microcalorimeters	374,987
Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity	314,002
Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accerlerators	317,705
High Power RF Window and Its Input Coupler Technology	375,000
Mercury Cadmium Telluride Detectors for Near Infrared Applications	300,000
Development of III-Nitride UV Detectors	374,980
Low Temperature, High Altitude Humidity Sensor	374,643
A Diode Laser Sensor for High Precision Measurement of Terrestrial CO_2 Sources and Sinks	374,879
A Generic Approach to Improved Semi-Solid Forming of Metals	374,445
High-Strain-Rate Superplastic Forging of Aluminum Alloys	375,000
Three Dimensional Si Imaging Array For Cold Neutrons	375,000
Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction	374,999

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,274,181
PHASE I	$1,296,204
Doppler Laser Radar for Non-Intrusive Liquid Metal Flow Characterization	98,896
Multi-Megawatt Circulator for TE_{01} Waveguide	100,000
Active Vibration Control of NLC Magnets	100,000
An Electrical Condition Monitoring Approach for Wire and Cable	98,170
Near-Infrared Spectropolarimetry for On-Line Measurement of Polymer Rheology	100,000
X-Ray Diagnostics for High-Temperature Superconductor Processing	100,000
On-Line Texture Diagnostics for Coated Conductor Manufacture	100,000
Real Time *In-Situ* Composition and Thickness Control System for Deposition of Superconducting Tape Films	100,000
Non-Invasive Techniques to Study Local Passivity Breakdown of Metal Alloys in Aqueous Media	99,365
Microelectrode Array for Electrochemical Sensing of Localized Corrosion	100,000
High Resolution Imaging System for Corrosion Measurement	100,000
Smart Phosphors for Turbine Engine Measurement and Life Prediction	99,773
Intelligent Probes for Enhanced Non-Destructive Determination of Degradation in Hot-Gas-Path Components	100,000
PHASE II (FIRST YEAR)	$700,000
Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells	375,000
Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire	325,000
PHASE II (SECOND YEAR)	$1,277,977
SunGuard: A Roofing Tile for Natural Cooling	374,949
High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content	300,000
Development of New Lossy Material for Cryogenic and Ambient Applications	228,028
An Advanced Avalanche-Photodiode Based Spectroscopic Radiation Imager	375,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$12,908,328
PHASE I	$3,986,919
Innovative Organic and Inorganic High-Pressure Laminate Insulation for Fusion and Superconducting Magnets	99,835
Inorganic-Organic Hybrid Materials: Diacetylene-Siloxanes as Radiation Resistant Electrical Insulator for Plasma Fusion Confinement Systems	99,999
High Conductivity, Low-Cost SiC/SiC Composites	99,997
Ultra-Thin Optical Diagnostic Filters for Plasma Wakefield Accelerators	99,817
A Tubular Filamented Dispersion Strengthened Powder (DSP) Alloy Core Nb_3Sn Superconductor	99,900

OFFICE OF SCIENCE (continued)

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)

DIVISION OF TECHNOLOGY RESEARCH (continued)

SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)

PHASE I (continued)

	FY 2001
X-Ray Initiated Epoxy Adhesive for Detector Assembly	100,000
Photonic Crystal Scintillating Fibers	99,997
Enhanced Efficiency Nanowire Photocathode for Large PMTs	100,000
Nanostructured Externally Cure-Initiated Thermally and Electrically Conductive Adhesives	99,999
Synthesis of Crystalline $Hg_xCd_{l-x}I_{2,}$ a New Material for Room Temperature X-Ray and Gamma-Ray Detectors	89,680
A Multi-Layered Ceramic Composite for Impermeable Fuel Cladding for Commercial Water Reactors	99,950
Superinsulation for Ductwork	100,000
Developing Desiccant Coatings for the Elastomer Bed for Optimal Enthalpy Exchange Ventilation	100,000
Novel Synthesis Method for Producing Spherical and Elongated Metallic Nanoparticles for Advanced Heat Transfer Nanofluids	100,000
Surfaced Functionalized Nanoparticles for Nanofluids	100,000
Recycling of Polystyrene Packaging from the Food Service Industry	100,000
Recycling of Coated Plastics Used in Automotive, IT and Commercial Applications	99,991
PBO Films as Templates for Production of High Efficiency Nanoporous Composite Membranes	99,978
Encapsulated Particles: Improved Catalyst for the Production of Methanol from CO	100,000
Two-Step Methane Conversion to Alkynes and Dienes	100,000
One-Step Process for Propylene Oxide Production Directly from Hydrogen, Oxyen and Propylene by Using a Dual-Function Nanoparticle Catalyst	100,000
Improved Buffered Substrates for YBCO Coated Conductors	100,000
Development of Textured Buffer Layer On Metal Tapes for Oxide Superconductors	99,953
Development of High-Temperature Cr-Based Intermetallic Alloys for Structural Applications	100,000
Enhanced Moly Silicide Intermetallic Alloys	99,987
Nano-Engineered Permanent Magnet Materials	100,000
Low Cost MesoCarbon Micro Bead Anodes for Lithium-Ion Batteries	100,000
High Retention Capacity Nanostructured Li_xFePO_4 Cathodes for Rechargeaable Li-Ion Batteries	100,000
A Novel Cathode Material for High Power Lithium Rechargeable Batteries	100,000
New Low-Cost Lithium Salts for Small and Full Size Rechargeable Batteries	100,000
Development of Low-Cost Salts for Lithium-Ion, Rechargeable Batteries	99,083
Novel Treatment of Power Plant Fly Ash for Use as Low-Cost Mercury Sorbent	99,753
High-Performance Carbon Materials for Ultracapacitors	99,925
Pyrolytic Mass Production of High Quality Carbon Nanotubes Using Advanced Catalysts Discovered by Integrated Catalysts Chips	100,000
Synthesis of Bulk Amounts of Double-Walled Carbon Nanotubes	100,000
Amorphous Coating for Protection of Austentic Steel in Coal-Fired Environments	100,000
Intermediate Temperature Solid Oxide Fuel Cell Development	99,079

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
PHASE I (continued)	
Laser Surface Modification for Improving Corrosion Resistance of Steels Used in Coal-Fired Power Systems	99,996
Novel Ceria-Based Materials for Low-Temperature Solid Oxide Fuel Cells	100,000
Nanostructured Anode Material for High Performance, Intermediate Temperature Solid Oxide Fuel Cell	100,000
PHASE II (FIRST YEAR)	$3,922,654
The Development and Demonstration of Reliable Adherent Metalization of AlN	375,000
Novel Lithium-Ion Conducting Polymer Electrolytes for Lithium-Ion Batteries	374,997
Synthesis of New Solid Polymer Electrolyte	374,999
Membranes for Reverse Organic-Air Separations	300,000
Hydrogen Recovery Process Using New Membrane Materials	300,000
New Boronated Amino Acids for Neutron Capture Therapy	268,028
Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials	300,000
Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate	355,000
A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection	375,000
In-Situ Electron Beam Processing for Radio Frequency Cavities	300,000
An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire	299,630
High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling	300,000
PHASE II (SECOND YEAR)	$4,998,755
Thermally Stable Catalysts for Methane Combustion	300,000
Improved Precursors for Oxygen-Selective Membranes in Practical Devices for Methane Conversion	375,000
Supported Flat Plate Thin Films for Oxygen Separation	374,996
A New Radiation Resistant Epoxy Resin System for Liquid Impregnation Fabrication of Composite Insulation	374,990
Advanced Heat Sink Materials for Fusion Energy Device	375,000
Hybrid 3-D SiC/C High Thermal Conductivity Composites	375,000
Co-Processed Ceramic Insulation for High Field Accelerator Magnets	300,000
Improvement of High Field Performance and Reliability of Nb_3Sn Conductor by PIT Method	300,000
Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings	374,960
Large Area Filtered Arc Deposition of Carbon and Boron Based Hard Coatings	374,967
Meter Length YBCO Coated Conductor Development	375,000
Novel Catalyst for CH_4-CO Conversion	350,000
Flame Retardant Electrolytes for Li-Ion Batteries	373,842
Nonflammable Lithium-Ion Battery Electrolytes	375,000

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
DIVISION OF TECHNOLOGY RESEARCH (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES	$798,541
PHASE I	$798,541
Development of a Universal Plastic Resin Composition Sensor for Whole Parts and Reground Mixtures	100,000
Sol-Gel Derived Neutron Detector Using a Lithiated Glass	98,880
Development of an Ultra-Bright Electron Source for Scanning Transmission Electron Microscopy	99,863
High Resolution Hybrid MCP Detector for Thermal Neutrons	100,000
Large Format MicroFiber Detector for Low Energy Neutrons	100,000
Pixel-Cell Neutron Detector and Read-Out System Meeting Requirements of Present and Future Neutron Scattering Facilities	100,000
Novel Neutron Detector for High Rate Imaging Applications	99,921
Smart Condition Monitor for High Temperature Turbine Blades	99,877
SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM	$1,249,963
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$449,996
PHASE I	$199,996
Advanced Membrane Technology for Biosolvents	100,000
CO_2 Removal from Natural Gas	99,996
PHASE II (SECOND YEAR)	$250,000
Thin-Film Fiber Optic Sensors for Power Control and Fault Detection	250,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$199,967
PHASE I	$199,967
Multiplexed Optical Fiber Chemical Sensor Arrays for Real-Time In Situ Monitoring of the Localized Corrosion Environment	99,967
Neutron Scattering Instrumentation for Measurement of Melt Structure	100,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$500,000
PHASE I	$500,000
Virtual-Impact Particle Sizing for Precursor Powders of Nb_3Sn and Bi-2212 Superconductors	100,000
Innovative Processing Methods for Superconducting Materials	100,000
Oxide Dispersed Nanofluids for Next Generation Heat Transfer Fluids	100,000
Integrated Remanufacturing/Materials Recovery Process for Optimum Recycling of Plastics	100,000
Plasma Spraying of $Nd_2Fe_{12}B$ Permanent Magnet Materials	100,000

OFFICE OF SCIENCE (continued)

	FY 2001
OFFICE OF FUSION ENERGY SCIENCES	$8,600,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,600,000
Vanadium Alloy and Insulating Coating Research	2,900,000
Theory and Modeling	700,000
Ferritic/martensitic Steel Research	1,600,000
SiC/SiC Composites Research	1,400,000
Plasma Facing Materials Research	2,000,000

OFFICE OF SCIENCE

The Office of Science (SC) advances the science and technology foundation for the Department and the Nation to achieve efficiency in energy use, diverse and reliable energy sources, a productive and competitive economy, improved health and environmental quality, and a fundamental understanding of matter and energy. The Director of Science is responsible for six major outlay programs: Basic Energy Sciences, Fusion Energy, Health and Environmental Research, High Energy and Nuclear Physics and Computational and Technology Research. The Director also advises the Secretary on DOE physical research programs, university-based education and training activities, grants, and other forms of financial assistance.

The Office of Science mainly conducts materials research in the following offices and divisions:

Office of Basic Energy Sciences - Division of Materials Sciences and Engineering
Office of Advanced Scientific Computing Research - Division of Advanced Energy Projects and Technology Research
Office of Biological and Environmental Research - Medical Sciences Division
Office of Fusion Energy - Division of Advanced Physics and Technology

Materials research is carried out through the DOE national laboratories, other federal laboratories, and grants to universities and industry.

OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences (BES) supports basic research in the natural sciences leading to new and improved energy technologies and to understanding and mitigating the environmental impacts of energy technologies. The BES program is one of the Nation's foremost sponsors of fundamental research in broad areas of materials sciences, chemical sciences, geosciences, biosciences, and engineering sciences. The BES program underpins the DOE missions in energy and the environment, advances energy-related basic science on a broad front, and provides unique national user facilities for the scientific community.

The program supports two distinct but interrelated activities: 1) research operations, primarily at U.S. universities and 11 DOE national laboratories and 2) user-facility operations, design, and construction. Encompassing more than 2,400 researchers in 200 institutions and 17 of the Nation's premier user facilities, the program involves extensive interactions at the interagency, national, and international levels. All research activities supported by BES undergo rigorous peer evaluation through competitive grant proposals, program reviews, and advisory panels. The challenge of the BES program is to simultaneously achieve excellence in basic research with high relevance to the Nation's energy future, while providing strong stewardship of the Nation's research performers and the institutions that house them to ensure stable, essential research communities and premier national user facilities.

DIVISION OF MATERIALS SCIENCES AND ENGINEERING

The Division of Materials Sciences conducts a broad program of materials research to increase the understanding of phenomena and properties important to materials behavior that will contribute to meeting the needs of present and future energy technologies. The Division supports fundamental research in materials at DOE national laboratories and plans, constructs, and operates national scientific user facilities needed for materials research. In addition, the Division funds over 230 grants, mostly with universities, on a wide range of topics in materials research.

Fundamental materials research is carried out at eleven DOE laboratories: Ames Laboratory at Iowa State University, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Environmental and Engineering Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories in New Mexico and California, and the Stanford Synchrotron Radiation Laboratory. The laboratories also conduct significant research activities for other DOE programs such as Energy Efficiency, Fossil Energy, Nuclear Energy, Environmental Management and Defense Programs. The Division of Materials Sciences and Engineering also funds the University of Illinois Frederick Seitz Materials Research Laboratory.

The performance parameters, economics, environmental acceptability and safety of all energy generation, conversion, transmission, and conservation technologies are limited by the discovery and optimization of the behavior and performance of materials in these energy technologies. Fundamental materials research seeks to understand the synergistic relationship between the synthesis, processing, structure, properties, behavior, performance of materials of importance to energy technology applications and recycling of materials. Such understanding is necessary in order to develop the cost-effective capability to discover technologically and economically desirable new materials and cost-competitive and environmentally acceptable methods for their synthesis, processing, fabrication, quality manufacture and recycling. The materials program supports strategically relevant basic scientific research that is necessary to discover new materials and processes and to eventually find optimal synthesis, processing, fabricating, and manufacturing parameters for materials. Materials Science research enables sustainable development so that economic growth can be achieved while improving environmental quality. Description of research supported by various elements of the materials program is presented below.

THEORETICAL CONDENSED MATTER PHYSICS

The Theoretical Condensed Matter Physics program is a diverse program that provides theoretical support for all relevant parts of the Materials Science program. Research areas parallel those in the experimental core research areas, including quantum dots, nanotubes and their properties, tribology at the atomic level, superconductivity, magnetism, and optics. A significant part of the portfolio consists of the development of advanced computer simulation algorithms, and fast codes to treat many particle systems. Research is conducted in 7 DOE laboratories, Ames, Argonne, Berkeley, Brookhaven, Los Alamos, the National Renewable Energy Laboratory, Oak Ridge and at 35 universities. An important component of the portfolio is the Computational Materials Science Network (CMSN) which brings together groups of scientists from DOE laboratories, universities, and to a lesser extent industry to solve materials problems requiring collaboration across disciplinary boundaries. The FY 2001 funding for this program is $16,124,000 and the DOE contacts are Manfred Leiser, (301) 903-4894, and Dale D. Koelling, (301) 903-2187.

EXPERIMENTAL CONDENSED MATTER PHYSICS

The portfolio consists of a broad-based experimental program in condensed matter and materials physics research with selected emphases in the areas of electronic structure, surfaces/interfaces, and new materials. It includes the development and exploitation of advanced experimental techniques and methodology. The objective is to provide the understanding of the physical phenomena and processes underlying the properties and behavior of advanced materials. It provides the technology-base support in condensed matter physics to energy technologies and contributes to the generic knowledge base in condensed matter and materials physics. The portfolio and scope are determined by opportunities, National Laboratory research expertise, and unsolicited research applications, as modified by programmatic requirements including scientific impact, materials needs, and energy technology requirements. Presently, the portfolio includes specific research thrusts in magnetism, semiconductors, superconductivity, materials synthesis and crystal growth, and photoemission spectroscopy. The portfolio addresses well-recognized needs, including understanding magnetism and superconductivity, the control of electrons and photons in solids, understanding materials at reduced dimensionality, the physical properties of large, interacting systems, and the properties of materials under extreme conditions. The FY 2001 funding for this program is $35,837,000 and the DOE contact is Jerry Smith, (301) 903-4269.

MATERIALS CHEMISTRY

The program addresses basic research on the synthesis, characterization, and chemical properties of materials to gain a more fundamental understanding of the effects of chemical reactivity on the synthesis and behavior of novel materials and structures. The portfolio includes research with particular emphases on surface and interfacial chemistry, nanoscience, polymer and organic materials, and solid state chemistry which underpin many energy related areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics and environmental chemistry. It includes investigations of novel materials including low-dimensional, self-assembled monolayers; cluster and nanocrystal-based materials; polymeric conductors; organic superconductors and magnets; complex fluids; biomolecular materials; and solid state neutron detectors. The research employs a wide variety of experimental techniques to characterize these materials including X-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and X-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as high-resolution magnetic resonance imaging (MRI) without magnets, neutron reflectometry, and atomic force microscopy of liquids. The FY 2001 funding for this program is $30,808,000 and the DOE contacts are Richard Kelley, (301) 903-6051 and Aravinda Kini (301) 903-3565.

MECHANICAL BEHAVIOR AND RADIATION EFFECTS

This activity focuses on the understanding of the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties. The objective is to understand the defect-property relationship at an atomic level. In the area of mechanical behavior, the research aims to advance understanding of deformation and fracture and to develop predictive models for design of materials having prescribed mechanical behavior. In the area of radiation effects, the research aims to advance understanding of mechanisms of amorphization (transition from crystalline to a non-crystalline phase), predict and suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by ion implantation. The FY 2001 funding for this program is $15,286,000 and the DOE contact is Yok Chen, (301) 903-4174.

NEUTRON AND X-RAY SCATTERING

Basic research in condensed matter and materials physics using neutron and X-ray scattering capabilities primarily at major BES-supported user facilities. Research is aimed at achieving a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials, and the relationship of these structures and excitations to the physical properties of materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena and behavior under environmental variables such as temperature, pressure, and magnetic field. Development of neutron and X-ray instrumentation for next generation sources. The FY 2001 funding for this program is $31,682,000 and the DOE contact is Helen Kerch, (301) 903-2346.

STRUCTURE AND COMPOSITION OF MATERIALS

Structure and composition of materials includes research on the arrangement and identity of atoms and molecules in materials; specifically the development of quantitative characterization techniques, theories and models describing how atoms and molecules are arranged, and the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces and precipitates. Advancing the state of the art of electron beam micro characterization methods and instruments is an essential element in this portfolio. Four electron beam user centers are operated at ANL, LBNL, ORNL, and the Frederick Seitz MRL at the University of Illinois. The FY 2001 funding for this program is $33,767,000 and the DOE contact is Altaf Carim, (301) 903-4895.

PHYSICAL BEHAVIOR

Physical behavior refers to the electronic, chemical, microstructural or other response of a material to an applied stimulus. The research in this portfolio aims to understand, predict and control physical behavior of materials by developing scientifically rigorous models for the response of materials to environmental stimuli such as temperature, electromagnetic field, chemical environment, and proximity of surfaces or interfaces. Basic research topics supported include modeling of materials behaviors, electrochemistry and corrosion, high-temperature materials performance, superconductivity, photovoltaics, and fuel cells. The FY 2001 funding for this program is $16,449,000 and the DOE contact is Robert Gottschall, (301) 903-3978.

SYNTHESIS AND PROCESSING SCIENCES

Synthesis and Processing Science includes research on understanding and developing innovative ways to make materials with desired structure, properties or behavior. Examples include atomic and molecular self-assembly to create new materials; nanostructured materials that mimic the structure of natural materials; new approaches to the processing of materials to improve properties or behavior; and welding and joining of materials. Since this research often requires specialized, high-purity materials that are not commercially or otherwise available, the Materials Preparation Center at the Ames Laboratory is operated for the purposes of developing methods, fabricating research grade materials, and providing these materials to the research community. The FY 2001 funding for this program is $12,801,000 and the DOE contacts are Tim Fitzsimmons, (301) 903-9830, and Bassem Armaly, (301) 903-4062.

ENGINEERING RESEARCH

Engineering Sciences includes research in the development of engineering principles to make scientific advances in materials practicable; in nanotechnology and microsystems; in multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. The FY 2001 funding for this program is $17,352,000 and the DOE contacts are Tim Fitzsimmons, (301) 903-9830, and Bassem Armaly, (301) 903-4062.

EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH

Basic research spanning the entire range of programmatic activities supported by the Department within the Office of Science in states that have historically received relatively less Federal research funding. The DOE designated EPSCoR states are Alabama, Alaska, Arkansas, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, and the Commonwealth of Puerto Rico. EPSCoR is managed in the Materials Science and Engineering Division within BES. The FY 2001 funding for this program is $7,685,000 and the DOE contact is Matesh Varma, (301) 903-3209.

NATIONAL USER FACILITIES

Basic Energy Sciences (BES) is responsible for the planning, construction, and operation of many of the Nation's most sophisticated research facilities, including third-generation synchrotron light sources and high-flux neutron sources as well as specialized facilities for microcharacterization, materials synthesis and processing, combustion research, and ion beam studies. These facilities are unmatched in the world in their breadth of capabilities and number of scientific users. BES facilities have enormous impact on science and technology, ranging from the structure of superconductors and biological molecules to the development of wear-resistant prostheses, from atomic-scale characterization of environmental samples to elucidation of geological processes, and from the production of unique isotopes for defense applications and cancer therapy to the development of new medical imaging technologies.

BES research facilities serve over 4,500 researchers from universities, industry, and government laboratories each year. These users conducted forefront research in physics, materials sciences, chemical sciences, earth sciences, structural biology, engineering, medical and other sciences. The costs for the construction and the safe, user-friendly operation of these world class facilities are substantially beyond the capability of individual academic and private industrial research laboratories. They are made available to all qualified users from academia, industry, and both DOE and non-DOE government laboratories, most generally without charge for non-proprietary research that will be published in the open literature.

The research facilities permit the Nation's science and technology enterprise to have access to research instruments that are required for world-competitive forefront research that would not otherwise be possible. Included amongst the numerous honors and distinctions to the research that has been carried out at the BES national user facilities was the 1994 Nobel Prize in Physics, shared by Dr. Clifford G. Shull, who carried out pioneering investigations in neutron scattering at Oak Ridge National Laboratory. All of the BES national user facilities have been constructed within cost, on schedule, and with rigorous compliance to all environmental, safety and health regulations. Further information about the National User Facilities can be found in "Scientific Research Facilities," published by the U.S. Department of Energy; available from the Office of Basic Energy Sciences, (301) 903-3081. The FY 2000 funding for this program is $283,217,000.

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

DIVISION OF TECHNOLOGY RESEARCH

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

206. **ADVANCED PROCESSING TECHNIQUES FOR TAILORED NANOSTRUCTURES IN RARE-EARTH PERMANENT MAGNETS (AL 01 02)**
$40,000
DOE Contact: Samuel J. Barish (301) 903-2917
AL Contact: Matthew Kramer (515) 294-0276

High-energy product (BH)max permanent magnets have enabled critical size and weight reduction in direct-current electric motors with an accompanying increase in energy efficiency. Nd-Fe-B based magnets are currently the clear choice for high-value commercial applications. Two classes of magnets are produced from these alloys. While the anisotropic (textured) magnets possess the highest (BH)max, they are limited to critical applications because of their high cost. Bonded magnets made from rapidly solidified alloys have significantly lower (BH)max; but in addition to lower cost of production, they offer the ability to produce net shape magnets and may easily be incorporated in larger motors resulting in considerable energy savings. While considerable progress has been made in controlling the rapid solidification process to reproducibly fabricate high-energy product magnet materials, advances have been largely empirical with limited fundamental understanding. This project supports the DOE mission in advanced synthesis and materials characterization technologies.

Recent developments in high-speed imaging techniques have documented a number of problems regarding the stability of the melt pool during melt spinning, and they provide the tools to address these problems in a systematic manner. A particularly severe problem is the ability of the alloy to wet the quench wheel. When the melt pool fails to wet the quench wheel, the lack of a stable pool will result in lower yield and inhomogeneous solidification of the fraction that contacts the quench wheel. The objective of this project is to determine the factors controlling wettability, including composition, impurities, and heat flow, using imaging techniques. In addition, procedures for processing digital images will be developed so that they may be transferred to the industry partner. The imaging techniques and the resulting enhanced control of processing will also be applied to producing anisotropic rapidly solidified permanent magnet powders. Such powders have the potential to increase the (BH)max of bonded magnets by a factor of four.

Keywords: Permanent Magnets, Anistropic Magnets, Bonded Magnets (Bh)max, Rapid Solidification Process, High-Speed Imaging Techniques, Quench Wheel, Anisotropic Rapidly Solidified Permanent Magnet Powders

207. **IMPROVED MATERIALS FOR SEMICONDUCTOR DEVICES (PNL 98 17)**
$117,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNL Contact: Suresh Baskaran (509) 375-6483

The increasingly higher performance required of semiconductor devices has resulted in a need for new materials to reduce the capacitance between metal conductor lines (interconnects) on semiconductors. The ability of a material to reduce capacitance losses is defined by its dielectric constant, and the development of interlevel dielectric materials with much lower dielectric constants than what is currently available is the focus of considerable attention within the semiconductor industry. In addition to improving electrical performance (power consumption, signal speed, and propagation noise), such materials offer the potential of significant reductions (about $500M annually) in fabrication costs for semiconductors. The project will develop mesoporous silica dielectric films. The controlled, highly porous structure of these films make them good candidates to obtain the types of properties the semiconductor industry is seeking in low k dielectrics. Pacific Northwest National Laboratory (PNNL) will focus on the design and synthesis of the new materials, including pore design, pore characterization, surface modification, and initial process development. SEMATECH will be responsible for extensive characterization of film performance and evaluation in relation to interconnect processing for semiconductors. SEMATECH hopes to identify low k dielectric materials capable of being utilized by its member companies in the manufacture of higher performance semiconductor devices. DOE missions will benefit through an improved understanding of mesoporous materials that also have energy-related applications in catalysis and sensing, and environmental applications in chemical separations. Experiments have been initiated to increase film thickness and minimize surface topography due to the spin coating process. Using nuclear reaction analysis and the Rutherford backscattering facility at the Environmental Molecular Sciences Laboratory, porosity was determined for surfactant-based films with a range of porosity from approximately 20 percent to about 60 percent. Ideally, from both performance and integration standpoints, films should contain high porosity with isolated pores. Therefore, PNNL researchers have also begun investigation of a synthesis approach for films with closed porosity using new soluble pore-formers.

Keywords: Semiconducting Devices, Interconnects, Silica Dieletric Film, Sematech

208. **DEVELOPMENT OF HIGH-TEMPERATURE SUPERCONDUCTING WIRE USING RABITS COATED TECHNOLOGIES (ORNL 97 02)**
$30,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: David K. Christen (423) 574-6269

High-temperature superconducting (HTS) materials hold promise for greatly improved energy efficiency in a number of power applications related to the production, distribution, storage, and utilization of electric energy. This project is directed at developing a new route to the fabrication of high-temperature superconducting wires for such power applications. The approach is based upon a recent breakthrough, referred to as RABiTS (Rolling Assisted Biaxially Textured Substrates), at the Oak Ridge National Laboratory (ORNL). The approach exploits the growth of crystalline biaxially-aligned coatings on long-length oriented metal tapes that are produced by simple thermomechanical processing. The achievement of biaxial texture is essential for the transport of large, loss-free electric currents, especially in the presence of magnetic fields. In the RABiTS approach, passivating “buffer” layers are deposited by electron beam and sputter deposition, and HTS coatings are deposited by electron-beam evaporation. The project is determining the scientific and technical feasibility of making long-length coated conductors that can provide operating characteristics that are currently unattainable by electrical conductor, including present prototype HTS tapes that utilize the “power-in-silver-tube” fabrication approach. ORNL research focuses on both the simplification and optimization of oxide buffer layers on reactive metals in general, and specifically is developing a simplified ex situ approach to the co-evaporation and processing of the superconductor coatings. Recent advances at ORNL using this approach have resulted in short-segment prototype conductors with critical current densities of over a million amps/cm at liquid nitrogen temperature. 3M is actively developing the scale-up of these techniques for the production of long-length tapes in a “continuous” process. 3M has established experience base in high-rate deposition of many materials in manufacturing technologies. Southwire is the leading U.S. manufacturer of utility wire and cable and is a retailer of under ground transmission lines capable of 2-5 times the power transfer into urban areas, without the need for additional rights-of-way and without significant losses to resistance. Other applications, such as power transformers, motors, current limiters, and magnetic energy storage, are projected to produce markets of tens-of-billions of dollars per year. This project supports DOE's mission to develop high-temperature superconductors.

Keywords: High Temperature Supeconducting Materials, Superconducting Wire, Rabits Technolgy Fabrication, Reactive Metals, Magnetic Energy Storage, Power Transformers and Motors, Current Limiters

209. **DEVELOPMENT OF BISMUTH-BASED SUPERCONDUCTING WIRE WITH IMPROVED CURRENT CARRYING AND FLUX PINNING PROPERTIES (ANL 99 15)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Victor Maroni (630) 252-4547

Progress in the commercialization of electric power equipment fabricated with high temperature superconducting materials has been limited by performance issues associated with the maximum achievable engineering critical current density, J_e, in long-length composite conductor. One of the most advanced conductors available today for such applications is the silver-clad $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$ (called Ag/Bi-2223) composite in multifilament form. However, the Je of Ag/Bi-2223 at 77 K in magnetic fields of 1 Tesla or more is not presently adequate for most types of motors, generators, transformers, current limiters, and related power system components. Research is aimed at investigating two new pathways to fabricate the next generation of improved bismuth-based superconducting wire. One pathway is focused on the controlled growth of strong flux pinning centers in Ag/Bi-2223 filaments by the implementation of special heat treatment procedures. These create a transient thermodynamic state that promotes the growth of selected second phase nanocrystallites having the correct size, shape, and spatial distribution to induce strong inter- and intra-granular flux pinning. The second pathway involves reducing the c-axis blocking layer gap (between CuO_2 planes) in layered bismuth cuprates by demonstrating fabrication of the silver-clad $(Bi,Pb,Cd)_1Sr_2Ca_1Cu_2O$ (M-1212) along lines that have been developed for Ag/Bi-2223. The "in-principle" advantage of M-1212 over Bi-2223 stems from the shorter (by ~4 D) blocking gap in M-1212 due to fewer atomic layers in the c-axis repeat unit. From preliminary work, there are existing laboratory scale indications that both pathways can lead to significant improvement in the performance of bismuth-based high temperature composite conductors. The project extends DOE commitments in characterization and design of advanced materials for the acceleration of superconducting technologies to US markets.

Keywords: Superconducting Materials, Silver-Clad $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$

210. **LIGHT EMISSION PROCESSES AND DOPANTS IN SOLID STATE LIGHT LIGHT SOURCES (LBNL 97 13)**
$11,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Eugene Haller (510) 486-5294

Light emitting diodes (LEDs) functioning in the red and infrared have been manufactured in large quantities since the 1960s. However, until very recently, only very inefficient and dim LEDs were available in the green and, especially, in the blue. Although there are a handful of semiconducting materials with sufficiently wide bandgaps to function in principle in the blue region of the spectrum, fundamental material properties and limitations have prevented bright and efficient diodes from being made. Recently, breakthroughs in the heteroepitaxial growth of gallium nitride (GaN) and its alloys with indium and aluminum have changed the blue and green LED technology outlook. Formerly, it was believed that III-V nitride layers had too high a defect density to function as LEDs. Nevertheless, a Japanese company (Nichia) has developed a family of blue and green LEDs based on GaN that are bright and efficient. For the last three years, Japanese companies have been manufacturing and selling blue GaN LEDs in bulk quantities. This project is a collaboration with HP, the leading U.S. producer of LEDs, to investigate the fundamental light-emitting mechanism in GaN-based LEDs. HP is providing GaN and InGaN layers and structures grown with their metal-organic chemical vapor deposition (MOCVD) equipment. Joint work is being performed in four technical areas: (1) Doping-related strain effects in GaN and InGaN epitaxial layers (2) Metal/GaN contacts (3) Localization properties of dopants and defects, and (4) Carrier transport in layers and devices. In the first technical area, it has been shown that compressive film stress and Si concentration, which were found to be positively correlated in previous work, could be varied independently by appropriate changes in growth conditions. This is of considerable importance to HP, because reliable production of thick GaN layers had been limited by cracking induced by the Si dopant. In work related to the localization and transport topics, optical measurements have been performed in diamond anvil cells with p-doped GaN single crystals, GaN, AlGaN, and InGaN single layers, and GaN/InGaN multilayer structures. These results are being used to understand the mechanism of light production in III-V nitrides supporting DOE's mission in materials research.

Keywords: Light Emitting Diodes, Red and Infrared Hetero-Epitaxial, Blue and Green LEDS, GAN

211. **DEVELOPMENT OF BUFFER LAYERS SUITABLE FOR DEPOSITION OF THICK SUPERCONDUCTING YBCO LAYERS BY A POST-DEPOSITION ANNEALING PROCESS (BNL 98 05)**
$125,000
DOE Contact: Samuel J. Barish (301) 903-2917
BNL Contact: M. Suenaga (516) 344-3518

The goal of this project is to develop a textured buffer layer on top of a metallic substrate, e.g., a textured Ni, which is compatible with the Brookhaven National Laboratory method of fabricating thick YBCO films, a post-deposition annealing method. In order to accomplish this, the project has started: (1) the purchase and installation of a textured measurement attachment to an existing X-ray apparatus (This makes it possible to determine the degree of the texture of the buffer layer as well as the substrate and YBCO layers.), and (2) testing of the chemical compatibility of CeO_2 with YBCO layers at the high temperature required for the formation of YBCO layers. A texture measuring attachment to a X-ray diffractometer was purchased and was installed such that a texture analysis of the rolled tapes, the buffer, or the superconducting films can be determined. This unit has been delivered and installed, and the process of a final acceptance of the unit is being performed. Since the post-deposition annealing process for growing thick (>5 μm) YBCO involves heat treating YBCO precursor films in a moist atmosphere at high temperatures (>725° C), it is important to select a buffer layer material which does not interfere with the growth of YBCO. In order to study this, the project has initially deposited an YBCO precursor film on a CeO_2 buffered single crystalline $LaAl0_3$ and heat treated it to form an YBCO layer on top of the CeO_2. Note that CeO_2 is a well-known buffer layer which is used in conjunction with pulsed laser deposition of YBCO. Although a significant reaction takes place between the YBCO and CeO_2 layers if they are heat-treated above 750˚C, the reaction appears to be sufficiently minimized by keeping the reaction temperature below 735˚C. A further study is being conducted to see the extent of the reaction, and other possible candidates for the buffer materials are being examined. If this project is successful, the superconducting tapes will be used in electrical utility systems, greatly increasing the efficiency of power transmission. This project supports DOE's mission through increased energy efficiency.

Keywords: Superconducting Oxides, Buffer Layers, Deposition of Thick Film, YBCo Buffer Layers, Electrical Utility Systems

212. **INTERPLAY BETWEEN INTERFACIAL AND DIELECTRIC AND FERROELECTRIC BEHAVIORS OF BARIUM STRONTIUM TITANATE THIN FILMS (PNL 99 08)**
$278,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNL Contact: Scott Chambers (509) 376-1766

Barium strontium titanate (BST) and related materials are entering commercial use for integrated circuit manufacture as conventional materials reach their fundamental limits. BST films have capacitance, leakage, and related electrical properties that surpass integrated circuit device requirements. One of the most important steps towards understanding the interplay between interfacial properties and dielectric and ferroelectric behaviors of BST ($Ba_{1-x}Sr_xTiO_3$) is the growth of high quality BST films on Si substrates. Successful epitaxial growth of crystalline BST on Si(001) is thought to require the formation of a two-dimensional interfacial silicide layer involving either Ba or Sr as the initial step. Bulk thermodynamics suggests that this thin silicide layer is required to stabilize the interface. The goal of the project is to address two specific issues of significant concern in BST thin-film technology: (1) the effect of interfacial chemistry and stress on the dielectric and ferroelectric properties of BST thin films, and (2) ferroelectric behavior at the nano-scale level. Research is focused on preparation, isolation, and characterization of an ultrathin silicide layer using Sr as the alkaline earth metal. Si(001)-(2x1) surfaces were prepared in ultra high vacuum (UHV) by rapid desorption of the native oxide layer. These surfaces were exposed to Sr from an effusion cell in an oxide MBE chamber as a function of evaporation rate, substrate temperature, and total dose. The resulting interfaces were characterized during growth with reflection high-energy electron diffraction (RHEED), and after growth with low-energy electron diffraction (LEED), X-ray photoemission (XPS), and x-ray photoelectron diffraction (XPD). Additionally, the team is initiating STM investigations to further elucidate this interface structure. Physical and electrical testing of these structures have been performed to determine interface roughness, interface layer formation, interface state density, dielectric properties (permittivity, leakage, etc.), and stability vs. post-growth processing. This project supports DOE's commitment to basic energy sciences in fostering the synthesis, processing, and characterization of advanced materials.

Keywords: BST Thin Films, Dielectric, Ferroelectric Materials, Interfacial Chemistry

213. **EFFICIENCY IMPROVEMENT OF NITRIDE-BASED SOLID STATE LIGHT-EMITTING MATERIALS (LBNL 01 04)**
$20,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Eicke Weber (510) 642-0205

During the last 30 years, the market for illumination with light-emitting diodes (LEDs) has grown rapidly. In 2000, the total worldwide LED component market was $2.9 billion. For example, LEDs are used to illuminate signs, electronic components, auto interiors, cell-phones, and signals. High-brightness (HB) LEDs became available during the last decade. In particular, GaN-based LEDs were developed to obtain light emission across the entire visible spectrum. It has been demonstrated that HB LEDs can be used for general lighting. However, they have not yet penetrated the general illumination market to any significant degree. Today, this market penetration is feasible, and it is the goal of this project to optimize performance aspects of GaN-based HB LEDs as required for applications in general lighting. This project supports the DOE mission in design of advanced materials.

Specifically, this project will attempt to understand the fundamental mechanism of radiative carrier recombination in group-III nitride thin films, emitting in the green, blue, and ultraviolet region. The issue is of concern for LumiLeds Lighting because it is crucial for its development of devices with improved light emission efficiency. Scientifically, the project will determine the indium content and its atomic-scale distribution, local measurements of the piezoelectric fields, and modeling of the impact of the piezoelectric field and the indium distribution on the emission efficiency of devices. To date, the mentioned properties of the III-nitrides are the focus of worldwide ongoing investigations, but they remain poorly understood. The team at LBNL has developed new technical approaches to study the underlying problems and it will use centers of excellence to conduct the novel experiments. These new experiments include transmission electron microscopy with unprecedented resolution, sensitivity, and precision and a newly-designed photoluminescence setup that is capable of uniquely relating strain-induced effects to light emission.

Keywords: Light-Emitting Diodes, Radiation Carrier Recombination, Piezoelectric Fields, Transmission Electron Microscopy

214. **ADVANCED COMPUTATIONAL MODELS AND EXPERIMENTS FOR DEFORMATION OF ALUMINUM ALLOYS – PROSPECTS FOR DESIGN (PNL 99 07)**
$278,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNL Contact: M.A. Khaleel (509) 375-2438

Dislocations are the basic lattice line defects in crystalline materials, with defect densities as high as 1015/m^2. This project aims at understanding their collective and complex nonlinear dynamical behavior by merging a set of highly sophisticated experiments, using computer aided, massive numerical analyses, and experimental data. The project impacts future computational and experimental advances in dislocation theory and elevates prospects for predictive alloy properties control. One motivation for this work is to characterize fabrication and durability characteristics of aluminum tailor welded blanks in order to demonstrate their viability for high volume, low cost stamped automotive panels and structures. Finite Element Modeling is being used to formulate accurate constitutive relations to allow complete description of material response during manufacture. Application of this research to manufacture and design of existing and new lightweight Al materials supports DOE's initiatives in high performance computing.

Keywords: Aluminum Alloys, Dislocation Phenomena, Predictive Properties Control

215. **NEAR-FRICTIONLESS CARBON COATINGS (ANL 98 03)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Ali Erdemir (630) 252-6571

Numerous industrial applications involve the use of mechanical devices containing components that slide or roll against one another. The efficiency and durability of these components are often limited by the friction and wear properties of the materials used to fabricate the components. For example, Diesel Technology Company (DTC) and Stirling Thermal Motors (STM) develop advanced energy conversion systems and engine components that will contribute significantly to reducing oil imports and improving air quality by reducing engine emissions. Fuel injection systems being designed and developed by Diesel Technology for use in heavy-duty diesel engines will require tighter tolerances to run on low-lubricity fuels at higher operating pressures needed to achieve emissions and efficiency goals. Since materials used in current fuel injection systems will not survive under these aggravated conditions, new materials and/or coatings are needed. Similarly, Stirling engines being designed by Stirling Thermal Motors will operate under tribological conditions (e.g., speeds, temperatures, loads, and working fluids) not commonly encountered, and will require advanced materials, coatings, and lubricants to ensure long-term durability. Argonne will work with Front-Edge Technologies (FET) to commercialize Argonne's technology for fuel injection systems and Stirling engine components being developed by DTC and STM. The objectives of this project are to: (1) advance the basic understanding of the physical/chemical and tribological processes controlling the friction and wear behavior of the new carbon films (2) demonstrate the ability of these coatings to improve the friction and wear performance of materials and components being developed by Diesel Technology and Stirling Thermal Motors, and (3) demonstrate that the coating technology can be scaled-up to coat large numbers of components on a cost-competitive basis. If successful, the NFC technology will have a significant impact not only on the technology being pursued by DTC and STM, but also in other applications found in the aerospace, biomedical, and manufacturing sectors. It builds on expertise at Argonne in tribology, coatings, and materials characterization. This project supports DOE missions in advanced materials and sustainable environments, reducing U.S. dependence on foreign oil imports, and improving U.S. air quality. This project won an R&D 100 Award in 1998.

Keywords: Carbon Coatings, Friction and Wear, Fuel Injection, New Materials, Coatings, Tribology

216. **FUNDAMENTAL SCIENTIFIC PROBLEMS IN MAGNETIC RECORDING (ORNL 01 04)**
$40,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: Thomas Schulthess (865) 574-4334

The project will address fundamental science problems confronted by the magnetic recording industry. Design of magnetic readers and magnetic media requires atomic-scale engineering of nanometer-scale magnetic heterostructures. Presently, designers of such devices must work with badly blurred vision because they cannot determine the structures at the necessary atomic scale. This project supports the DOE mission of advancing basic scientific understanding of materials.

The project team will develop atom probe techniques and technology that will allow the designers to obtain images of magnetic multilayers with atomic-scale resolution. The ever-decreasing size of magnetic bits requires higher coercivity media to prevent thermal fluctuations from affecting the stored information. Higher coercivity media will require that the writer has higher magnetization to reverse the bits. A fundamental study of magnetism in layered structures will be undertaken with the objective of developing a simple understanding of the limits to the saturation magnetization and of techniques for increasing it. Finally, a fundamental study of the exchange bias effect that is crucial for pinning one of the magnetic layers in recording heads, and magnetic memory devices based on the giant magnetoresistance effect, will be undertaken. If any of these three objectives are achieved, there will be a huge potential positive impact on the magnetic recording industry.

Keywords: Magnetic Readers, Atom Probe Techniques, Higher Coercivity Media, Saturation Magnetization, Exchange Bias Effect, Giant Magnetoresistance Effect

217. **NANOMETER CHARACTERIZATION AND DESIGN OF MOLECULAR LUBRICATION FOR THE HEAD-DISK INTERFACE (LBNL 98 10)**
$189,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Miquel Salmeron (510) 486-6704

Information recording density in magnetic storage (hard disks) is currently increasing at an annual rate greater than 60 percent. In the quest for ever higher performance, the trend in the industry is toward even smaller head-to-disk spacing. This project will attempt to characterize and design molecular lubrication for the head-disk interface (HDI). The goal of this project is to design advanced lubricants with properties tailored for the next generation of magnetic storage devices. The read head of a hard disk "Flies" within 10 nanometers of the disk surface, which is protected from damage during accidental contacts by an approximately 2 nanometer thick lubricating film. Although current film thickness is now less than the length of one lubricant molecule, industry standard characterization methods, based on optical techniques, are limited to micron-scale lateral resolution. Liquids exhibit unique physical properties when confined between surfaces separated by molecular dimensions, which have been used to develop a scanning polarization-force microscopy technique that is applicable to ultra-thin liquid films. This is the first non-invasive technique capable of imaging the structure of liquid films with approximately 50 nanometer lateral resolution and sub-nanometer normal resolution. The unique characterization methods developed at LBNL will be used to correlate nanoscale structure and properties with microscale engineering measurements and to develop and verify the performance of optimized, tailored HDI lubricants. The techniques developed at LBNL for the nanometer scale characterization of ultra-thin liquid films and droplets will be applied to determine the actual nanoscale structure, properties, and response to local contacts of head-disk interface lubricants used to identify critical performance parameters, with the final goal of designing an HDI lubricant with optimized wetting and spreading properties tailored for future generations of ultra-high density storage devices. This project supports the DOE mission in the application of basic research developments in materials sciences to new technologies.

Keywords: Characterization and Design, Molecular Lubrication, Magnetic Disk Storage, Advanced Lubricants, Thick Lubricating Films, Nanoscale Structures

218. **AN ADVANCED HARD CARBON PLASMA DEPOSITION SYSTEM WITH APPLICATION TO THE MAGNETIC STORAGE INDUSTRY (LBNL 98 16)**
$210,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Andre Anders (510) 486-6745

The goal of this project is to develop a novel plasma deposition system used to coat computer hard disks and read/write heads with ultra-thin, diamond-like carbon films that can be implemented on an industrial scale. The project will combine the commercial and basic research strengths of CSC and Lawrence Berkeley National Laboratory, respectively, to develop next generation, filtered arc deposition equipment. Project objectives include: couple the plasma source and macro-particle filter to complete macro-particle suppression; improve plasma transmission (hopefully double the rate compared to present efforts); trap macro-particles within the filter; and design a compact system that can be directly plugged into existing sputter coating facilities. The system will be reasonably priced and able to coat large areas. It is anticipated that the technology developed in this project will become a key tool for next generation high-density magnetic storage media, a multi-billion dollar market in which U.S. companies currently maintain a market leadership position. The coating system is of vital interest to the U.S. computer industry. Many of the top names in the magnetic storage industry have voiced their support for a filtered cathodic arc system for advanced carbon coating. The project supports the DOE mission in advanced materials, specifically synthesis and processing by ions and plasmas.

Keywords: Plasma Deposition System, Arc Deposition Equipment, Macroparticle Deposition, High Density Magnetic Storage Coatings

219. **INTERFACIAL PROPERTIES OF ELECTRON BEAM CURED COMPOSITES (ORNL 99 08)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: Christopher Janke (423) 574-9247

Electron Beam curing of composites and adhesives is a nonthermal, nonautoclave curing process which offers substantially reduced manufacturing costs and curing times, improvements in part quality and performance, reduced environmental and health concerns, and improvements in material handling, as compared to conventional thermal curing. As satisfactory properties of electron beam cured composites are achieved, U.S. industry expects rapid implementation of these materials for making better, less expensive, and lightweight airplanes, spacecraft, and automobiles. Previous research on electron beam cured composites has shown that interface dependent properties, such as composite interlaminar shear strength, are generally lower than those of high performance, autoclave cured composites. A primary objective of this project is to determine the chemical, physical, and/or mechanical mechanisms responsible for poor adhesion between carbon fibers and epoxy resins subjected to electron beam processing. Another important objective is to optimize electron beam compatible carbon fiber surface treatments, chemical agents, modified radiation curable epoxy resin systems, and improved fabrication and processing methods for producing electron beam cured composites having excellent interfacial properties. Currently, work is focused on characterization of the carbon fiber-epoxy resin interface and identification of the critical radiation processing parameters that influence the properties of electron beam cured composites. Additionally, various chemical agents, including coupling agents and reactive finishes, which are specifically designed to improve the fiber-resin adhesion properties, are being evaluated. The project complements DOE investments in advanced materials research, and research on energy efficiency and environmental stewardship.

Keywords: Electron Beam Processing, Electron Beam Cured Composites and Adhesives

220. **PHOTOCATALYTIC METAL DEPOSITION FOR NANOLITHOGRAPHY (ANL 99 13)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Tijana Rajh (630) 252-3542

A major technical impediment for the development of mesoscopic scale electronic devices is obtaining molecular scale conducting patterns. Based on the parameters that are optimized in highly efficient photochemical energy conversion in natural photosynthesis, Argonne National Laboratory has developed a new mask-less photoelectrochemical method for depositing conductive metal patterns with nanometer scale precision. This technology will enable the rapid prototyping and manufacturing of mesoscopic electronics and offers the potential of low-cost small batch manufacturing and unparalleled levels of electronic integration. This new technology is being used to fabricate miniaturized (ultimate resolution limit of 1 nm) and rugged electrical interconnects and biomolecular electronic devices on any surface or in solution. This project will enable the 3-D integration of passive and active components of mesoscopic integrated conformal electronics. In addition, the technology provides a unique advantage compared to other electronic technologies, because the semiconductor substrate (precursor) can also perform active function in the bioelectronic device. Conductor precursors, semiconductor metal oxide nanoparticles modified with chelating agents, that bind metal cations (copper, silver, and gold), will be synthesized. Biological templates will be used to self-assemble conductor precursors in order to achieve spacial resolution via photocatalysis. The fast photoresponse of semiconductor nanodots also provides high time resolution. Based on a fundamental understanding of electron transfer reactions in this biomimetic approach, precursor formulations will be developed and characterized for photoelectrochemical response, redox stability, and mechanical properties. Precursors will be deposited on a range of substrates (silicon, glass, plastic, metals, ceramics, etc.) or in solution. Conductive patterns formed by catalytic semiconductor assisted solid state deposition of copper, silver, or gold will be studied as a function of nanoparticle size, reduction technique, and nanoparticle-chelate association complex. Interconnects and biomolecular assemblies will be studied to ascertain morphology, function, and 3-D characterization as a function of processing methodology. The technology developed in this project is an extension of DOE's efforts to promote characterization of materials useful to nanotechnology.

Keywords: Metal Deposition, Nanolithography, Self Assembly, Photocatalysis

221. **LOW-COST, HIGH-PERFORMANCE YBCO CONDUCTORS (ORNL 01 06)**
$40,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: Parans Paranthaman (865) 574-5045

The successful demonstration of high-performance YBCO (YBCO) coated conductors by various institutions has generated great interest around the world. This project will support the DOE mission in energy efficiency.

The objective of this project is to develop material science and technology necessary for YBCO coated conductors on biaxially textured, nonmagnetic, high-strength substrates. Fundamental studies of the growth of oxide buffers on these nonmagnetic substrates will be conducted. The research goal is to also develop both vacuum and nonvacuum processes to deposit compatible buffers at high rates. These novel substrates will be the foundation or template upon which the American Superconductor Corporation will apply YBCO using its proprietary trifluoroacetate (TFA) solution process. Applications of these superconducting wires include high-efficiency motors, compact generators, underground transmission lines, oil-free transformers, and superconducting magnetic storage systems for smoothing voltage fluctuations in the power grid. The Rolling Assisted Biaxially Textured Substrates (RABiTS) process developed at ORNL will be utilized. ORNL and ASC have reported a very high J_c of 1.9 MA/cm^2 at 77K and self-field on YBCO films grown by their TFA solution process on standard RABiTS architecture of CeO_2 (sputtered)/YSZ (sputtered)/Gd_2O_3 (solution)/nickel. However, before scaling up to fabricate long conductors in a reel-to-reel configuration, several fundamental issues will be addressed. Nickel is magnetic, which means significant alternating-current losses, and is also mechanically soft. Hence, the first issue to be addressed is the development of mechanically strong, nonmagnetic, biaxially textured, alloy substrates. The deposition of an epitaxial oxide buffer layer on an nickel-alloy substrate is non-trivial due to the tendency of alloying elements in nickel to form nonepitaxial oxides on the surface of the substrate. The second issue to be addressed is the development of a suitable buffer layer stack for growth of high-J_c YBCO films. The high number of buffer layers increases the complexity of fabrication and cost of the conductor. A third objective is to simplify the buffer layer stacks. Because radio frequency magnetron sputtering has limited deposition rates, the fourth issue to be addressed is the investigation of higher rate processes for the fabrication of epitaxial oxide buffer layers on the nonmagnetic substrates. In this project, solutions for critical roadblocks will be addressed to possibly accelerate the development and commercialization of low-cost, YBCO high-temperature superconducting wires.

Keywords: Oxide Buffers, Trifluoroacetate Solution Process, RABiTS, Nickel Alloy Substrate, Radio Frequency Magnetron Sputtering

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

222. **NANOFABRICATION OF ADVANCED DIAMOND TOOLS (LBNL 01 03)**
$34,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Othon Monteiro (510) 486-6159

This project will investigate and develop fabrication processes for diamond tools and evaluate these tools in actual micromachining operations. The primary use of these tools will be for the repair of masks used in semiconductor processing. No technology is presently available for the repair of defects in masks to be used for the next generations (critical dimension of 0.13 mm and below). Nanomachining can be used for such repairs, and it is regarded as the only technique capable of repairing masks for deep ultraviolet lithography. The diamond tools will be manufactured by plasma-assisted chemical vapor deposition (CVD) of diamond on preformed molds, which are etched off after the deposition is completed. Silicon processing technology will be used to prepare the molds to be filled with diamond. Diamond is the most promising material for such tools because of its superior mechanical properties and wear resistance. This project supports the DOE mission in advanced materials.

The major objective of this project is the development of diamond tools (tips) to be used in micromachining and nanomachining operations using scanning-probe technology. The primary application of these tools will be in the repair of masks for the semiconductor industry. Industry and government groups, such as International Sematech, regard mask repair as absolutely critical to the ability to continue to advance semiconductor performance and device density. LBNL is interested in expanding the applications of CVD diamond to the manufacturing of microsize and nanosize mechanical, electronic, or optical devices. General Nanotechnology is directly interested in bringing the CVD diamond technology to the mask repair tools to be used in the lithography of circuits in the next several generations (critical dimensions below 130 nm). The project team intends to develop a manufacturing process to produce reliable and reproducible diamond tools and fully characterize these tools with regard to their performance in mask repair. The manufacturing process will be based on plasma-assisted CVD on prefabricated molds; for some special applications, final shaping processes will also be developed. The manufacturing process shall be capable of preparing those tool-bits on 4-in. silicon wafers, with diamond deposition rates of 1 to 2 µm/h, which is sufficient to guarantee the economic feasibility of the fabrication technique. In addition, the process shall be able to prepare tools (diamond tips) with different angles of attack and tip radii down to 2 nm. Mechanical toughness and hardness should be optimized, and wear rates of the most common materials used in lithographic masks shall be fully characterized, as well as the wear rate of the tools.

Phase I (Introductory Studies) has been completed. The major parameters affecting nucleation density are the existence of seed layer and the application of bias voltage. A diamond deposition process that makes use of the former has been developed at LBNL and has been used to prepare the initial samples. Implementation of the capability of biasing the substrate is being implemented to the existing diamond deposition chamber: design of the required components (electrodes and vacuum feedthroughs) is under way, and selection and purchase of the power supply are the next steps. The nucleation density achieved with the current process (seed layer) is sufficient to produce continuous (pin-hole free) diamond films with a thickness below 100 nm. Implementation of bias-enhanced nucleation is desired mostly for the capability of producing highly textured diamond films. Such films are smoother than conventional polycrystalline films. Phases II and III are also progressing at the planned rate. The development of techniques for preparing molds on silicon wafers has been successful. The shift from using conventional silicon to silicon-on-insulator has allowed greater reproducibility in mold and cantilever fabrication. Pyramid molds are currently being fabricated and used to test the diamond deposition process. Concurrently, the scanning-probe instrument that will be used for the evaluation of these nanotools has been installed in LBNL, and final software development is under way to allow the project to begin collecting data on tool performance and wear.

Keywords: Semiconductor Processing, Deep Ultraviolet Lithography, Silicon Processing Technology, Micromachining, Chemical Vapor Deposition, Silicon Wafers, Nucleation Density, Pyramid Molds

223. **IONICALLY CONDUCTIVE MEMBRANES FOR OXYGEN SEPARATION (LBNL 97 03)**
$35,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Steven J. Visco (510) 486-5821

There is currently a large need for solid state gamma The global market for industrial oxygen is estimated at $20 billion annually. The dominant technology for the production of commercial oxygen is cryogenic distillation. The high capital equipment costs for cryogenic O_2 separation limits this technology to large installations. Accordingly, industrial suppliers of oxygen are highly motivated to develop technologies that can satisfy increasing demand for oxygen through smaller scale plants. One approach under development elsewhere is the use of mixed ionic-electronic ceramics; when such ceramic electrolytes are exposed to compressed air on one side and ambient pressure on the other, oxygen diffuses through the mixed conductor from the compressed side to the low pressure side due to the chemical potential gradient of oxygen across the membrane. The drawback to this technology is the need for a compressor, which raises issues of noise and reliability. Another problem is that permeation delivers ambient pressure oxygen. In contrast, we propose the efficient electrolytic extraction of oxygen from air using novel thin-film structures consisting of high strength ionic membranes supported on porous, catalytic electrodes. Using this technology, high purity O_2 can be electrochemically pressurized as an integral part of the separation process. The simplicity of operation of an electrolytic O_2 generator promises high reliability as well as low cost. Still, to survive as a commercial process, this approach must be cost-competitive to cryogenic production of O_2. The key to success is highly efficient operation (low power consumption) of the device along with low fabrication costs. Power losses in the electrolytic oxygen cell will be related to ohmic losses across the electrolyte membrane, charge transfer polarization at the electrode/electrolyte interfaces, and mass transfer polarization across the electrodes. The LBNL approach addresses the above issues in such a way that both scientific and technical success are likely. The LBNL team has initiated preparation of porous substrates suitable for colloidal deposition. High temperature furnaces are being installed for sintering of bilayer structures suitable for high oxygen flux in an electrolytic oxygen generator. LBNL is working closely with the industrial partner to ensure maximum productivity of this collaborative effort. This research supports the DOE mission in materials research and applications.

Keywords: Oxygen, Membranes, Separation, Ceramic Electrolytes, Catalytic Electrodes, Oxygen Generators

224. **ALLOY DESIGN AND DEVELOPMENT OF CAST CR-W-V FERRITIC STEELS FOR IMPROVED HIGH-TEMPERATURE STRENGTH FOR POWER GENERATION APPLICATIONS (ORNL 01 08)**
$33,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: R. L. Klueh (865) 574-5111

Economic and environmental concerns demand that the power-generation industry develop higher efficiency fossil-fired power plants. Higher efficiency requires higher operating temperatures. The initial objective for the hottest sections of new systems is 593°C, eventually increasing to 650ºC. High-temperature materials research and development for power-generation systems has been neglected in the United States in recent years, while industry-government consortiums in Europe and Japan have pursued aggressive development programs. For the U.S. power industry to stay competitive, a program to develop advanced high-temperature materials is required. To operate at higher temperatures, new ferritic steel castings with improved properties are required for rotors, casings, and pipes. ORNL has developed several wrought Cr-W-V steels with 3–9% chromium, 2–3% tungsten, and 0.25% vanadium plus minor amounts of additional elements with the strength and toughness required for some of these applications. However, cast alloys behave differently from wrought alloys, and no data are available on the steels in the cast condition. This project will use these new steels as a basis to design and develop castings with the strength and the microstructural behavior suitable for future power systems. This project supports the DOE mission in advanced materials.

Modeling studies will be integrated with microstructural and mechanical properties studies on as-cast structures and thermally aged and creep-tested material that can be used as feedback on the stability of the microstructure at projected operating temperatures to guide alloy design for properties optimization. Results will be compared to a baseline of commercial castings and service-exposed steel from equipment used by the power-generating industry. The combination of microstructural/mechanical properties data and modeling studies to develop a scientific understanding of the underlying mechanisms of microstructural evolution during melting, casting, processing, and service should lead to the efficient design and implementation of improved power-plant steels. This project will combine the scientific expertise and research facilities of a DOE laboratory with the technical expertise on existing materials and manufacturing approaches of GE Power Systems, a world leader in the development and manufacture of power-generating equipment. Although the project will not eliminate the lead currently held by Europe and Japan in this field, a successful conclusion to the project would once again put DOE in the forefront of development of advanced steels for elevated-temperature service. This was the case when modified 9Cr-1Mo steel was developed at ORNL, a steel presently being used by researchers in Europe and Japan as the base for comparison of the new steels being developed there.

Keywords: Fossil-Fired Power Plants, Melting, Casting, High-Temperature Materials, Rotors, Wrought Alloys

225. **HIGHLY DISPERSED SOLID ACID CATALYSTS ON MESOPOROUS SILICA (PNL 97 28)**
$48,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNNL Contact: Charles Peden (509) 376-5117

This project will develop new materials optimized for use as solid acid catalysts by coupling the advanced characteristics of mesoporous silica with the superacidic properties of tungstophosphoric acid and sulfated zirconia. The surface of mesoporous silica will be functionalized to accommodate the dispersion of tungstophosphoric acid and sulfated zirconia. This approach should produce a new class of highly active, shape selective, and robust solid superacid materials. The novel catalysts will be tested with the alkylation and isomerization reactions in the bench and pilot scale testing unit. The goal is to exceed the performance characteristics of existing solid superacid catalysts, thereby enabling the chemical and petrochemical industries to replace homogeneous acid catalysts. This will contribute to DOE’s mission to reduce environmental impacts in the energy sector. Homogeneous acid catalysts such as sulfuric acid and aluminum chloride are currently used to catalyze many industrially important reactions. Although these homogeneous acid catalysts are efficient, they are not environmentally benign and create many operational problems. These problems can be mitigated with solid acid catalysts. Tungstophosphoric acid and sulfated zirconia are two solid acid catalysts with super acidity. Low catalytic efficiency is the common problem with these two catalysts. In addition, it is difficult to disperse tungstophosphoric acid on supports due to its large cluster size,, and sulfated zirconia generally suffers rapid deactivation. These problems can be minimized with the superior characteristics of mesoporous silica. This work will enhance understanding of how the mesoporous support properties and acid grafting strategy influence reactivity, yields, selectivity, thermal stability, coking, and regeneration of the solid acid catalysts. In FY 1998, efforts were conducted to define the specific catalyst properties of interest. Synthesis and functionalization of the mesoporous silica supports was also initiated.

Keywords: Solid Acid Catalyst, Mesoporous Silica, Tungstophosphoric Acid, Sulfated Zirconia

226. **DEVELOPMENT OF A HIGH-EFFICIENCY ROTARY MAGNETOCALORIC REFRIGERATOR PROTOTYPE (AL 99 02)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
AL Contact: K. A. Gschneidner, Jr. (515) 294-7931

Magnetic refrigeration is based on the magnetocaloric effect—the ability of some materials to heat up when magnetized and cool when removed from the magnetic field. Using these materials as refrigerants would provide an environmentally friendly alternative to the volatile liquid chemicals, such as chlorofluorocarbons and hydrochloro-fluorocarbons, used in traditional vapor-cycle cooling systems. The new materials, have two advantages over existing magnetic coolants: they exhibit a giant magnetocaloric effect, and their operating temperature can be tuned from about 30K (-400˚F) to about 290K (65˚F) by adjusting the ratio of silicon to germanium—the more germanium, the lower the temperature. The efficiency of the new materials make magnetic refrigeration even more competitive with conventional gas-compression technology by replacing complex and costly superconducting magnets with permanent magnets in refrigerator designs. The elimination of superconducting magnets may also open the way for small-scale applications of this technology, such as climate control in cars and homes, and in home refrigerators and freezers. In addition, G. Schneidner says, “the discovery may also launch totally new applications for efficient refrigerators at very low refrigeration powers since gas compression technology cannot be scaled down to such low cooling powers and since thermoelectric cooling is very inefficient (30 times less than magnetic refrigerants).” The first gadolinium-based magnetic refrigerator has been demonstrated. The refrigerator has been operating for over six months, which far exceeds the few hours or days of operation recorded by similar units. In addition, the unit has achieved cooling power 20 to 1,000 times greater than previous units. Currently, the team is working to find practical means of processing the new materials to construct and test a variety of magnetic refrigerators, which span temperatures from 20K (-425˚F) to 300K (80˚F) and have cooling powers ranging from one watt to 50,000 watts. The project transfers DOE’s investments in materials research to research in energy efficiency through reduction in operating costs in air conditioning and refrigeration.

Keywords: Magnetocaloric Effect, Magnetocaloric Refrigeration, Gadolinium-Based Magnetic Materials

227. **DIRECT CASTING OF TITANIUM ALLOY WIRE FOR LOW-COST AEROSPACE AND AUTOMOTIVE FASTENERS (PNL 99 02)**
$278,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNNL Contact: Mark Smith (509) 376-2847

Current wire production methods require large ingots to undergo multiple reduction steps until a diameter of 7mm or less is obtained. The reduction steps are energy intensive, require expensive equipment, and result in the generation of scrap materials and undesirable etchant and lubricant waste. Economic analysis indicates that direct casting of a titanium wire to a diameter slightly larger than the desired final product, followed by relatively small final reduction steps, will result in significant savings to the aerospace industry and other titanium wire/rod users.

The direct casting process involves the use of a titanium core wire to serve as the carrier substrate onto which titanium will be cast and solidified at high feed rates. The objectives of the project include the development of unique atmosphere-controlled casting equipment, the application of thermal models to optimize the design and operation of the casting process, and extensive materials testing and characterization to establish the capability of the process to match properties produced by conventional processing. The project extends DOE investments in materials characterization to develop process technologies which further reduction of industrial waste emissions.

Keywords: Titanium Alloy Wire, Casting Processes

228. **NONCONSUMABLE METAL ANODES FOR PRIMARY MAGNESIUM PRODUCTION (ANL 98 05)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Michael J. Pellin (630) 252-3510

This project will develop a nonconsumable metal anode to replace consumable carbon anodes now used in commercial electrolysis cells for primary magnesium production. The use and manufacture of consumable carbon anodes, which must be constantly replaced, is costly, energy consuming, and occasions unwanted gaseous emissions such as CO_2 and HCl. In support of the DOE mission for energy efficient, environmentally sound industrial processes, ANL has identified certain metal alloys that are promising candidate materials for nonconsumable anodes. Such alloys form self-limiting surface oxide films that are thin enough to allow current to pass, yet thick enough to prevent attack of the underlying metal. These alloys are dynamic in that the more volatile, reactive components segregate to the surface at rates sufficient to reform the protective film as it dissolves in the chloride melt. The project will form surface films on candidate alloys and investigate them using surface analysis instruments and techniques. Promising alloys will be tested as anodes in bench-scale magnesium electrolysis cells. Cell operation will be monitored and interrupted at key points to remove the anode and investigate its surface film. If desirable, the anode film thickness and strain during electrolysis in specially designed cells will be studied. Alloys identified as optimal will be subject to long-term bench-scale tests by Dow Chemical Company, and then tested in full-scale cells at Dow's production facility in Freeport, Texas. Successful completion of this work will result in increased U.S. competitiveness and lower magnesium prices which would, for example, allow magnesium to be used more widely in the transportation sector, resulting in lower costs there. If successful, stable anodes would reduce the operation cost of making magnesium by 20-30 percent and eliminate the emission of CO_2 and other halocarbon gases during magnesium production by eliminating the need for carbon anodes, now used to produce magnesium electrolytically. Moreover, this work will illuminate the mechanisms associated with film formation on alloys. An understanding of these mechanisms (e.g., surface segregation, near surface diffusion) will provide the basis for developing a new class of corrosion resistant materials that can find application in harsh chemical environments, for example as nonconsumable anodes for aluminum production.

Keywords: Magnesium Production, Metal Anodes, Metal Alloy, Co_2 Emissions, Corrosion Resistant, Film Formation

229. **DEVELOPMENT OF ELECTROLYTE AND ELECTRODE MATERIALS FOR RECHARGEABLE LITHIUM BATTERIES (BNL 98 04)**
$74,000
DOE Contact: Samuel J. Barish (301) 903-2917
BNL Contact: Xiao-Qing Yang (516) 344-3663

Enhancing performance, reducing cost, and replacing toxic materials by environmentally benign materials are strategic goals of DOE in lithium battery research. Development of new electrolyte materials, aza and boron based anion receptors as additives, organic lithium salts, and plasticizers is aimed at enhancing the conductivity and lithium transference number of lithium battery electrolytes and reducing the use of toxic salts in these electrolytes. The objective of the project is to develop these electrolyte and cathode materials for rechargeable lithium batteries, especially for lithium ion and lithium polymer batteries. The research targets optimization of boron-compound-based composite electrolytes, and synthesis of new lithium salts and plasticizers for polymer and polymer gel electrolytes. Characterization of cathode materials will be carried out utilizing the National Synchrotron Light Source. *In situ* X-ray absorption and X-ray diffraction techniques, developed at BNL, will be used to probe the relationship between performance and the electronic and structural characteristics of intercalation compounds such as $LiNiO_2$, $LiCoO_2$, and $LiMn_2O_4$ spinel. New cathode materials, such as $LiNi_{0.8}Co_{0.2}O_2$, $LiNi_{0.8}Co_{0.2-z}Al_zO_2$, and $LiNi_{0.7}Mg_{0.125}Ti_{0.125}O_2$, have also been studied. These results will be used to guide new material selection and quality control procedures. Successful research will result in the development of less expensive and more environmental friendly lithium battery materials for commercial applications.

The project marshals DOE's investment in basic materials research to promote economically and environmentally desirable new processes and materials for energy use.

Keywords: Lithium Based Materials, Lithium Batteries

230. **OPTIMIZED CATALYSTS FOR THE CRACKING OF HEAVIER PETROLEUM FEEDSTOCKS (LBNL 99 01)**
$300,000
DOE Contact: Samuel J. Barish (301) 903-2927
LBL Contact: Gabor Somorjai (510) 486-4831

Catalysts lower the energy required for chemical reactions to proceed and are widely used in petroleum refining and chemical manufacturing. The useful lifetime and, thus, the value of an industrial catalyst are limited by a process known as deactivation in which the efficiency of the catalyst declines over time. Understanding the deactivation process is essential for developing new catalysts with longer useful lifetimes. There are two industrially important catalytic systems under study at present. In the first study, zeolite-based catalysts are being developed to remove undesired sulfur compounds from gasoline. The goal of this project is to evaluate the mechanism by which sulfur is adsorbed on the catalyst. Of particular interest is the identification of catalyst "active sites" that actually interact with the sulfur. This is done by spectroscopically monitoring the identity of the surface species under reaction conditions. The second system under study is the "reforming" reactions of n-hexane and n-heptane with hydrogen that produce high octane gasoline by converting the reactants to benzene and toluene. Deactivation in these catalysts proceeds via "coking," the buildup and polymerization of carbonaceous reaction byproducts on the surface of the catalyst. The vibrational spectra of these byproducts will be obtained by UV-Raman spectroscopy for identification purposes. Ultraviolet excitation is required in this case to avoid interference from black body radiation from the hot catalyst material. Identification of problematic surface species will allow determination of the precise mechanism by which deactivation occurs in this system. These improvements will have a major impact on the efficiency of petroleum refining and gasoline production. The new surface science tools under development will have applicability to general studies in catalysis and surface science and support the DOE's mission in design and characterization of advanced materials.

Keywords: In-Situ Surface UV-Raman Spectroscopy, Catalytic Surfaces, Catalyst Deactivation, Zeolite Based Materials

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Fabrication of Polyimide Inertial Fusion Energy Target Capsules by a Fully Automated Process - DOE contact Gene Nardella, (301) 903-4956; Luxel Corporation contact Dan Wittkopp, (360) 378-4137

Sealed, High-Heat Capacity, Cable-in-Conduit Superconductors - DOE contact Warren Marton, (301) 903-4958; Superconducting Systems, Inc. contact Dr. Shahin Pourrahimi, (781) 642-6702

A Novel Reactive Processing Method to Join SiC Components for Fusion Applications - DOE contact Sam E. Berk, (301) 903-4171; Applied Thin Films, Inc. contact John Rechner, (847) 467-5235

Joining of Advanced SiCf/SiCm Composites for Fusion Energy Applications - DOE contact Sam E. Berk, (301) 903-4171; FM Technologies, Inc. contact Dr. Frederick M. Mako, (703) 425-5111

A High-Power, Ceramic, RF Generator and Extractor - DOE contact Jerry Peters, (301) 903-3233; Duly Research, Inc. contact Dr. David U. L. Yu, (310) 548-7123

Quasi-Optical Millimeter-Wave Accelerating Structure - DOE contact Jerry Peters, (301) 903-3233; Omega-p, Inc. contact George P. Trahan, (203) 458-1144

KA-Band RF Transmission Line Components for a High-Gradient Linear Accelerator - DOE contact Jerry Peters, (301) 903-3233; Omega-p, Inc. contact George P. Trahan, (203) 458-1144

A Novel Process for Producing Low Cost Sn-Ti Core Rods for Internal Tin Nb_3Sn - DOE contact Jerry Peters, (301) 903-3233; Paul D. Jablonski contact Dr. Paul D. Jablonski, (330) 305-0841

A Scalable APC Process with a Novel Pin Structure for High Field Magnets - DOE contact Jerry Peters, (301) 903-3233; Supercon, Inc. contact Terence Wong, (508) 842-0174

Enabling Technologies for Inline Heat Treatment of Nb_3Sn Precursor Cables Suited to Fabrication of Nb_3Sn Flexible Cables - DOE contact Jerry Peters, (301) 903-3233; Superconducting Systems, Inc. contact Dr. Shahin Pourrahimi, (781) 642-6702

A Method to Increase Current Density in a Mono Element Internal Tin Process Superconductor Utilizing ZrO_2 to Refine the Grain Size - DOE contact Jerry Peters, (301) 903-3233; Supergenics contact Bruce Zeitlin, (941) 349-0930

Hermetic Metallization of Aluminum Nitride for Radio Frequency Devices - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Sienna Technologies, Inc. contact Dr. Canan Savrun, (425) 485-7272

Detector Arrays Based on Fast Scintillators - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Adherent Technologies, Inc. contact Dr. Ronald E. Allred, (505) 346-1685

Thick Silicon Photodiodes for High Efficiency X- and Gamma-Ray Spectroscopy - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Photon Imaging, Inc. contact Dr. Bradley E. Patt, (818) 709-2468

High Density CZT Array Assembly Techniques - DOE contact Peter Kirchner, (301) 903-9106; Aguila Technologies, Inc. contact M. Albert Capote, (760) 752-1199

A Liquid-Desiccant Heating/Cooling System Powered by Solar Energy - DOE contact Lew Pratsch, (202) 586-1512; Ail Research, Inc. contact Dr. Andrew Lowenstein, (609) 452-2950

Truss-Integrated Thermoformed Ductwork - DOE contact Esher Kweller, (202) 586-9136; Steven Winter Associates, Inc. contact Marie Starnes, (203) 857-0200

Reactive Separation via a Hydrothermally Stable Hydrogen Selective Membrane - DOE contact Charlie Russomanno, (202) 586-7543; Media And Process Technology, Inc. contact Dr. Paul Liu, (412) 826-3721

Novel Membrane Reactor for the Desulfurization of Transportation Fuels - DOE contact Charlie Russomanno, (202) 586-7543; Trans Ionics Corporation contact Sandra C. Schucker, (281) 296-9210

Low-Cost Ceramic Modules Incorporating Palladium-Based Membranes for Dehydrogenation Reactions - DOE contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation contact Dr. Robert L. Goldsmith, (781) 899-4495

Low Emission Diesel Engines - DOE contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. contact Nadine Cragg-Lester, (302) 999-7996

Selective Adsorption Membranes for the Production of Enriched Air - DOE contact Charlie Russomanno, (202) 586-7543; ITN Energy Systems, Inc. contact Janet Casteel, (303) 285-5111

Treatment of Produced Water with Fouling-Resistant Nanofiltration Membranes - DOE contact Charlie Russomanno, (202) 586-7543; Membrane Technology And Research, Inc. (MTR) contact E. G. Weiss, (650) 328-2228

Low-Cost, Large-Membrane-Area Modules for Gas Separation - DOE contact Charlie Russomanno, (202) 586-7543; Membrane Technology And Research, Inc. (MTR) contact E. G. Weiss, (650) 328-2228

An Acoustically Enhanced Pervaporation Bioreactor (APB) - DOE contact Charlie Russomanno, (202) 586-7543; Montec Research contact Lawrence Farrar, (406) 723-2222

Novel Thin-Film Ceria Membrane Materials for Small-Scale Oxygen Generation Systems - DOE contact Brian Valentine, (202) 586-1739; Nextech Materials, Ltd. contact Dr. Scott L. Swartz, (614) 842-6606

Pyrolitic Boron Nitride Neutron Sensitive Direct Converter Layers - DOE contact Helen Kerch, (301) 903-2346; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (618) 926-1167

Novel Nanocomposite Anodes for Lithium-Ion Batteries - DOE contact Jim Barnes, (202) 586-5657; EIC Laboratories, Inc. contact Dr. R. David Rauh, (781) 769-9450

Novel Nano-Structured Catalyst for Steam Gasification of Carbonaceous Feedstocks - DOE contact Doug Archer, (301) 903-9443; Ceramem Corporation contact Dr. Robert L. Goldsmith, (781) 899-4495

Treated Silicate Sorbents for Mercury Removal from Flue Gas - DOE contact Barbara Carney, (304) 285-4671; ADA Technologies, Inc. contact Clifton H. Brown, (303) 792-5615

Control of Catalyst Poisons from Coal Gasifiers - DOE contact Bob Kornosky, (412) 386-4521; TDA Research, Inc. contact Michael Karpuk, (303) 940-2301

High-Temperature Highly-Efficient Ceramic Heat Exchanger - DOE contact Richard J. Dunst, (412) 386-6694; Ceramatec, Inc. contact Dale M. Taylor, (801) 978-2132

Integrated Membrane System for Upgrading Nitrogen-Rich Natual Gas - DOE contact Tony Zammerilli, (304) 285-4641; Membrane Technology And Research, Inc. (MTR) contact E. G. Weiss, (650) 328-2228

Zero-Emission Natural Gas Glycol Dehydrator System with Improved Drying Capacity - DOE contact Tony Zammerilli, (304) 285-4641; Membrane Technology And Research, Inc. (MTR) contact E. G. Weiss, (650) 328-2228

PHASE II (FIRST YEAR)

Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating - DOE contact George Seweryniak, (301) 903-0071; Ionic Systems, Inc. contact Constance Eve Teague, (408) 885-0800

Advanced Geothermal Optical Transducer (AGOT) - DOE contact Raymond J. LaSala, (202) 586-4198; LEL Corporation contact Mrs. Piedao H. Liucci, (201) 569-8641

Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape - DOE contact Helen Kerch, (301) 903-2346; Nova Scientific, Inc. contact Dr. Paul L. White, (508) 347-7679

Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors - DOE contact Charlie Russomanno, (202) 586-7543; Eltron Research, Inc. contact Eileen E. Sammells, (303) 530-0263

Affinity Ceramic Membranes with Carbon Dioxide Transport Channel - DOE contact Charlie Russomanno, (202) 586-7543; Media and Process Technology, Inc. contact Dr. Paul K.T. Liu, (412) 826-3721

Photocatalytic Membranes for Producing Ultrapure Water - DOE contact Charlie Russomanno, (202) 586-7543; Technology Assessment & Transfer, Inc. contact Mrs. Sharon S. Fehrenbacher, (410) 224-3710

Novel Membrane Reactor for Fischer-Tropsch Synthesis - DOE contact Charlie Russomanno, (202) 586-7543; CeraMem Corporation contact Dr. Robert Goldsmith, (781) 899-4495

Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron-Emission Tomography Imaging - DOE contact Prem Srivastava, (301) 903-4071; Nova R & D, Inc. contact Raymond B. Pifer, (909) 781-7332

Miniature Electrochemical Carbon Dioxide Detector - DOE contact Roger Dahlman, (301) 903-4951; Superior Sensing Solutions contact Michael J. Newman, (303) 702-1672

An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis - DOE contact Paul Bayer, (301) 903-5324; Lynntech, Inc. contact Dr. G. Duncan Hitchens, (979) 693-0017

Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys - DOE contact Richard Read, (412) 386-5721; Materials & Electrochemical Research (MER) Corp. contact Dr. R.O. Loutfy, (520) 574-1980

A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells - DOE contact Wayne Surdoval, (412) 386-6002; Materials and Systems Research, Inc. contact Dr. Dinesh K. Shetty, (801) 530-4987

Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications - DOE contact Richard Read, (412) 386-5721; Touchstone Research Laboratory, Ltd. contact Brian E. Joseph, (304) 547-5800

Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells - DOE contact Ronald J. Fiskum, (202) 586-9154; FuelCell Energy, Inc. contact Dr. Hans Maru, (203) 825-6006

Efficient Incandescent Lighting Based on Selective Thermal Emitters - DOE contact John Ryan, (202) 586-9130; Foster-Miller, Inc. contact Adi R. Guzdar, (781) 684-4239

'On Chip' Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications - DOE contact Alec Bulawka, (202) 586-5633; ARSECO contact Mrs. Marine Boyadzhyan, (818) 249-6362

Infrared Focal Plane Array with Fast Shuttering - DOE contact Eric Sander, (202) 586-5852; Princeton Scientific Instruments, Inc. contact John L. Lowrance, (732) 274-0774

Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single-Photon Sensitivity - DOE contact Eric Sander, (202) 586-5852; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Constellation Technology Corporation contact Charles Settgast, (727) 547-0600

Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors - DOE contact Jehanne Simon-Gillo, (301) 903-1455; IntraSpec, Inc. contact John Walter, (865) 483-1394

Micromachined Silicon, Large Area X-Ray Detector - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Physical Optics Corporation contact Gordon Drew, (310) 320-3088

Cost Reduction Techniques for Powder in Tube Niobium Tin Superconductors - DOE contact Jerry Peters, (301) 903-5228; Supercon, Inc. contact Elaine Tarkiainen, (508) 842-0174

Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets - DOE contact Jerry Peters, (301) 903-5228; Superconducting Systems, Inc. contact Dr. Shanin Pourrahimi, (781) 642-6702

Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout - DOE contact Michael P. Procario, (301) 903-2890; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal Thermal-to-Electric Converters - DOE contact Lisa C. Herrera, (301) 903-8218; Triton Systems, Inc. contact Ross Haghighat, (978) 250-4200

PHASE II (SECOND YEAR)

High-Temperature Oscillator and Digital Clock - DOE contact Raymond J. LaSala, (202) 586-4198; Linear Measurements, Inc. contact Robert Hatch, (619) 535-2172

Capacitors for Extreme Temperature Applications - DOE contact Gideon Varga, (202) 586-0082; Sigma Technologies International, Inc. contact Dr. Angelo Yializis, (520) 575-8013

A High Temperature MEMS Inclination Sensor for Geothermal Drilling - DOE contact Raymond J. LaSala, (202) 586-4198; Silicon Designs, Inc. contact John C. Cole, (425) 391-8329

High Efficiency Thermoelectric Power Conversion Device - DOE contact Jim Merritt, (202) 586-0903; Hi-Z Technology, Inc. contact Norbert Elsner, (619) 695-6660

Fast Repetitive Arc Free Current Limiting Circuit Breaker - DOE contact T. V. George, (301) 903-4957; UTRON, Inc. contact Dr. F. Douglas Witherspoon, (703) 369-5552

A High Current Very Low Cost $Niobium_3Tin$ Titanium Doped Conductor Utilizing A Novel Internal Tin Process, with Separate Stabilizing Elements Scalable To Modern Niobium Titanium Production Economics - DOE contact Jerry Peters, (301) 903-5228; Supergenics contact Bruce A. Zeitlin, (941) 349-0930

Automated Diamond Turning Lathe for the Production of Copper Accelerator Cells - DOE contact Jerry Peters, (301) 903-5228; DAC Vision, Inc. contact James W. Drain, (805) 684-8307

High Power Switch - DOE contact Jerry Peters, (301) 903-5228; Diversified Technologies, Inc. contact Michael A. Kempkes, (781) 275-9444

Adiabatic Forming of Copper Accelerator Cells for the NLC - DOE contact Jerry Peters, (301) 903-5228; LMC, Inc. contact Lennart J. Lindell, (815) 758-3514

Low Cost Support Structures, With New Advanced Composite Materials Tailored For Ultra-Stable Particle Tracking Detectors - DOE contact Michael P. Procario, (301) 903-2890; HYTEC, Inc. contact William O. Miller, (505) 662-0080

SQUID Susceptometers for Read Out of Magnetic Microcalorimeters - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Hypres, Inc. contact Dr. Elie Track, (914) 592-1190

Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Advanced Energy Systems, Inc. contact Anthony Favale, (516) 575-9345

Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accelerators - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Advanced Energy Systems, Inc. contact Anthony Favale, (516) 575-9345

High Power RF Window and Its Input Coupler Technology - DOE contact Jehanne Simon-Gillo, (301) 903-1455; AMAC International, Inc. contact Dr. Quan-Sheng Shu, (757) 269-5641

Mercury Cadmium Telluride Detectors for Near Infrared Applications - DOE contact Rick Petty, (301) 903-5548; Avyd Devices, Inc. contact Dr. Honnavalli R. Vydyanath, (714) 751-8553

Development of III-Nitride UV Detectors - DOE contact Rick Petty, (301) 903-5548; Avyd Devices, Inc. contact Dr. Honnavalli R. Vydyanath, (714) 751-8553

Low Temperature, High Altitude Humidity Sensor - DOE contact Rick Petty, (301) 903-5548; Nanomaterials Research Corporation contact Molly M. W. Kostelecky, (303) 702-1672

A Diode Laser Sensor for High Precision Measurement of Terrestrial CO_2 Sources and Sinks - DOE contact Roger Dahlman, (301) 903-4951; Physical Sciences, Inc. contact Dr. Byron David Green, (978) 689-0003

A Generic Approach to Improved Semi-Solid Forming of Metals - DOE contact Yok Chen, (301) 903-3428; Chesapeake Composites Corporation contact Dr. Alexander Brown, (302) 324-9110

High-Strain-Rate Superplastic Forging of Aluminum Alloys - DOE contact Yok Chen, (301) 903-3428; Materials Modification, Inc. contact Dr. T.S. Sudarshan, (703) 560-1371

Three Dimensional Si Imaging Array For Cold Neutrons - DOE contact Helen Kerch, (301) 903-2346; IntraSpec, Inc. contact John Walter, (423) 483-1859

Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction - DOE contact Carl Friesen, (208) 526-1765; Intelligent Optical Systems, Inc. contact Robert Lieberman, (310) 530-7130

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Doppler Laser Radar for Non-Intrusive Liquid Metal Flow Characterization - DOE contact Sam E. Berk, (301) 903-4171; Think Tank, Inc. contact Dr. Madhavan M. Menon, (865) 966-6200

Multi-Megawatt Circulator for TE_{01} Waveguide - DOE contact Jerry Peters, (301) 903-3233; Calabazas Creek Research contact Dr. Lawrence Ives, (408) 741-8680

Active Vibration Control of NLC Magnets - DOE contact Jerry Peters, (301) 903-3233; Energen, Inc. contact Dr. Chad H. Joshi, (978) 671-5400

An Electrical Condition Monitoring Approach for Wire and Cable - DOE contact Frank Ross, (301) 903-4416; BPW Incorporated contact Shelby J. Morris Jr., (757) 850-8679

Near-Infrared Spectropolarimetry for On-Line Measurement of Polymer Rheology - DOE contact Charlie Russomanno, (202) 586-7543; Brimrose Corporation Of America contact Diane C. Murray, (512) 303-2362

X-Ray Diagnostics for High-Temperature Superconductor Processing - DOE contact David Welch, (631) 344-3517; Aracor contact Ed LeBaker, (408) 733-7780

On-Line Texture Diagnostics for Coated Conductor Manufacture - DOE contact David Welch, (631) 344-3517; Microcoating Technologies contact Jeffrey C. Moore, (678) 287-2403

Real Time *In-Situ* Composition and Thickness Control System for Deposition of Superconducting Tape Films - DOE contact David Welch, (631) 344-3517; Structured Materials Industries, Inc. contact Dr. Gary S. Tompa, (732) 885-5909

Non-Invasive Techniques to Study Local Passivity Breakdown of Metal Alloys in Aqueous Media - DOE contact Kevin Zavadil, (505) 845-8442; Applicable Electronics, Inc. contact Alan M. Shipley, (508) 833-5042

Microelectrode Array for Electrochemical Sensing of Localized Corrosion - DOE contact Kevin Zavadil, (505) 845-8442; Faraday Technology, Inc. contact Dr. E. Jennings Taylor, (937) 836-7749

High Resolution Imaging System for Corrosion Measurement - DOE contact Kevin Zavadil, (505) 845-8442; Omega International Technology, Inc. contact Dr. Nand K. Gupta, (815) 344-5455

Smart Phosphors for Turbine Engine Measurement and Life Prediction - DOE contact Lane Wilson, (304) 285-1336; Ipitek contact Robert Downey, (760) 930-2220

Intelligent Probes for Enhanced Non-Destructive Determination of Degradation in Hot-Gas-Path Components - DOE contact Lane Wilson, (304) 285-1336; Jentek Sensors, Inc. contact Dr. Neil J. Goldfine, (781) 642-9666

PHASE II (FIRST YEAR)

Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells - DOE contact Wayne Surdoval, (412) 386-6002; Applied Thin Films, Inc. contact Derrick Calandra, (847) 467-6877

Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire - DOE contact Jerry Peters, (301) 903-5228; Microcoating Technologies contact Jeffrey Moore, (678) 287-2400

PHASE II (SECOND YEAR)

SunGuard: A Roofing Tile for Natural Cooling - DOE contact Terrence Logee, (202) 586-1689; Powerlight Corporation contact Thomas L. Dinwoodie, (510) 540-0550

High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content - DOE contact Jerry Peters, (301) 903-5228; Superconducting Systems, Inc. contact Minou Mossavat, (781) 642-6702

Development of New Lossy Material for Cryogenic and Ambient Applications - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Ceradyne, Inc. contact Howard George, (714) 549-0421

An Advanced Avalanche-Photodiode Based Spectroscopic Radiation Imager - DOE contact Kamalendu Das, (304) 285-4065; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Innovative Organic and Inorganic High-Pressure Laminate Insulation for Fusion and Superconducting Magnets - DOE contact Warren Marton, (301) 903-4958; Composite Technology Development, Inc. contact Dr. Naseem A. Munshi, (303) 664-0394

Inorganic-Organic Hybrid Materials: Diacetylene-Siloxanes as Radiation Resistant Electrical Insulator for Plasma Fusion Confinement Systems - DOE contact

Warren Marton, (301) 903-4958; Eltron Research, Inc. contact Eileen E. Sammells, (303) 530-0263

High Conductivity, Low-Cost SiC/SiC Composites - DOE contact Sam E. Berk, (301) 903-4171; Thor Technologies, Inc. contact Vicki Schwab, (505) 845-1245

Ultra-Thin Optical Diagnostic Filters for Plasma Wakefield Accelerators - DOE contact Jerry Peters, (301) 903-3233; Luxel Corporation contact Dan Wittkopp, (360) 378-4137

A Tubular Filamented Dispersion Strengthened Powder (DSP) Alloy Core Nb_3Sn Superconductor - DOE contact Jerry Peters, (301) 903-3233; Dsp Alloys contact Gordon G. Chase, (858) 274-9228

X-Ray Initiated Epoxy Adhesive for Detector Assembly - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Adherent Technologies, Inc. contact Dr. Donald Allred, (505) 346-1685

Photonic Crystal Scintillating Fibers - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Intelligent Optical Systems, Inc. contact Dr. Robert A Lieberman, (310) 530-7130

Enhanced Efficiency Nanowire Photocathode for Large PMTs - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Nanosciences Corporation contact Dr. John Steinbeck, (203) 267-4440

Nanostructured Externally Cure-Initiated Thermally and Electrically Conductive Adhesives - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Nanosonic, Inc. contact Dr. Richard O. Claus, (540) 953-1785

Synthesis of Crystalline $Hg_xCd_{l-x}I_2$, a New Material for Room Temperature X-Ray and Gamma-Ray Detectors - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Termomecanica contact Dr. Natacha DePaola, (518) 348-2084

A Multi-Layered Ceramic Composite for Impermeable Fuel Cladding for Commercial Water Reactors - DOE contact Madeline Feltus, (301) 903-2308; Gamma Engineering Corporation contact Herbert Feinroth, (301) 840-8415

Superinsulation for Ductwork - DOE contact Esher Kweller, (202) 586-9136; Aspen Systems, Inc. contact Dr. Kang P. Lee, (508) 481-5058

Developing Desiccant Coatings for the Elastomer Bed for Optimal Enthalpy Exchange Ventilation - DOE contact Ronald J. Fiskum, (202) 586-9154; Elastek, Inc. contact Dr. Anthony DeGregoria, (608) 238-6466

Novel Synthesis Method for Producing Spherical and Elongated Metallic Nanoparticles for Advanced Heat Transfer Nanofluids - DOE contact Glenn Strahs, (202) 586-2305; Mer Corp (Materials And Electrochemical Research) contact Dr. James Withers, (520) 574-1980

Surfaced Functionalized Nanoparticles for Nanofluids - DOE contact Glenn Strahs, (202) 586-2305; Tda Research, Inc. contact Michael E. Karpuk, (303) 940-2301

Recycling of Polystyrene Packaging from the Food Service Industry - DOE contact Charlie Russomanno, (202) 586-7543; Adherent Technologies, Inc. contact Dr. Ronald E. Allred, (505) 346-1685

Recycling of Coated Plastics Used in Automotive, IT and Commercial Applications - DOE contact Charlie Russomanno, (202) 586-7543; Metss Corporation contact Dr. Kenneth J. Heater, (614) 842-6600

PBO Films as Templates for Production of High Efficiency Nanoporous Composite Membranes - DOE contact Charlie Russomanno, (202) 586-7543; Foster-miller, Inc. contact Ross R. Olander, (781) 684-4305

Encapsulated Particles: Improved Catalyst for the Production of Methanol from CO - DOE contact Charlie Russomanno, (202) 586-7543; Apyron Technologies, Inc. contact Dr. Les Story, (678) 405-2702

Two-Step Methane Conversion to Alkynes and Dienes - DOE contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation contact Dr. Robert L. Goldsmith, (781) 899-4495

One-Step Process for Propylene Oxide Production Directly from Hydrogen, Oxyen and Propylene by Using a Dual-Function Nanoparticle Catalyst - DOE contact Charlie Russomanno, (202) 586-7543; Hydrocarbon Technologies, Inc. contact Alfred G. Comolli, (609) 394-3102

Improved Buffered Substrates for YBCO Coated Conductors - DOE contact David Welch, (631) 344-3517; American Superconductor Corporation contact Thomas M. Rosa, (508) 621-4265

Development of Textured Buffer Layer On Metal Tapes for Oxide Superconductors - DOE contact David Welch, (631) 344-3517; Ues, Inc. contact Francis F. Williams, Jr., (937) 426-6900

Development of High-Temperature Cr-Based Intermetallic Alloys for Structural Applications - DOE contact Linda Horton, (865) 574-5081; Multi-phase Services, Inc. contact Dr. Robert H. Tien, (865) 966-6878

Enhanced Moly Silicide Intermetallic Alloys - DOE contact

Linda Horton, (865) 574-5081; Powdermet, Inc. contact Andrew Sherman, (818) 768-6420

Nano-Engineered Permanent Magnet Materials - DOE contact Sam Bader, (630) 252-4960; Powdermet, Inc. contact Andrew J. Sherman, (818) 768-6420

Low Cost MesoCarbon Micro Bead Anodes for Lithium-Ion Batteries - DOE contact Jim Barnes, (202) 586-5657; Mer Corp (materials And Electrochemical Research) contact Dr. J.C. Withers, (520) 574-1980

High Retention Capacity Nanostructured Li_xFePO_4 Cathodes for Rechargeaable Li-Ion Batteries - DOE contact Jim Barnes, (202) 586-5657; Nanopowder Enterprises, Inc. contact Dr. Gary S. Tompa, (732) 885-1088

A Novel Cathode Material for High Power Lithium Rechargeable Batteries - DOE contact Jim Barnes, (202) 586-5657; T/j Technologies, Inc. contact Leslie Alexander, (734) 213-1637

New Low-Cost Lithium Salts for Small and Full Size Rechargeable Batteries - DOE contact Jim Barnes, (202) 586-5657; Techdrive, Inc. contact Dr. Robert Filler, (630) 291-3414

Development of Low-Cost Salts for Lithium-Ion, Rechargeable Batteries - DOE contact Jim Barnes, (202) 586-5657; Yardney Technical Products, Inc. contact Vince Yevoli, (860) 599-1100

Novel Treatment of Power Plant Fly Ash for Use as Low-Cost Mercury Sorbent - DOE contact Barbara Carney, (304) 285-4671; Physical Sciences, Inc. contact Dr. B. David Green, (978) 689-0003

High-Performance Carbon Materials for Ultracapacitors - DOE contact Ben Hsieh, (304) 285-4254; Advanced Fuel Research, Inc. contact Dr. Michael A. Serio, (860) 528-9806

Pyrolytic Mass Production of High Quality Carbon Nanotubes Using Advanced Catalysts Discovered by Integrated Catalysts Chips - DOE contact Ben Hsieh, (304) 285-4254; Intematix Corporation contact Dr. Young Yoo, (925) 631-9005

Synthesis of Bulk Amounts of Double-Walled Carbon Nanotubes - DOE contact Ben Hsieh, (304) 285-4254; Mer Corp (materials And Electrochemical Research) contact Dr. J. C. Withers, (520) 574-1980

Amorphous Coating for Protection of Austentic Steel in Coal-Fired Environments - DOE contact Richard J. Dunst, (412) 386-6694; Applied Thin Films, Inc. contact John Rechner, (847) 467-5235

Intermediate Temperature Solid Oxide Fuel Cell Development - DOE contact Lane Wilson, (304) 285-1336; Ceramatec, Inc. contact Dr. Michael Keene, (801) 978-2152

Laser Surface Modification for Improving Corrosion Resistance of Steels Used in Coal-Fired Power Systems - DOE contact Richard J. Dunst, (412) 386-6694; Karta Technology, Inc. contact Dr. G.P. Singh, (210) 582-3000

Novel Ceria-Based Materials for Low-Temperature Solid Oxide Fuel Cells - DOE contact Lane Wilson, (304) 285-1336; Nextech Materials, Ltd. contact Dr. Scott L. Swartz, (614) 842-6606

Nanostructured Anode Material for High Performance, Intermediate Temperature Solid Oxide Fuel Cell - DOE contact Lane Wilson, (304) 285-1336; Us Nanocorp, Inc. contact Dr. David Reisner, (860) 678-7561

PHASE II (FIRST YEAR)

The Development and Demonstration of Reliable Adherent Metalization of AIN - DOE contact Samuel Barish, (301) 903-2917; MER Corporation contact Dr. R.O. Loutfy, (520) 574-1980

Novel Lithium-Ion Conducting Polymer Electrolytes for Lithium-Ion Batteries - DOE contact Susan Rogers, (202) 586-8997; Eltron Research, Inc. contact Eileen Sammells, (303) 530-0263

Synthesis of New Solid Polymer Electrolytes - DOE contact Susan Rogers, (202) 586-8997; TPL, Inc. contact H.M. Stoller, (505) 342-4412

Membranes for Reverse Organic-Air Separations - DOE contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. contact Glenn Walker, (937) 252-8969

Hydrogen Recovery Process Using New Membrane Materials - DOE contact Charlie Russomanno, (202) 586-7543; Membrane Technology and Research, Inc. contact E.G. Weiss, (650) 328-2228

New Boronated Amino Acids for Neutron Capture Therapy - DOE contact Peter Kirchner, (301) 903-9106; BioNeutrics, Inc. contact Larry Tummel, (865) 675-5627

Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials - DOE contact Neil Rossmeissl, (202) 586-8668; Materials & Electrochemical Research (MER) Corp. contact Dr. J.C. Withers, (520) 574-1980

Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate - DOE contact Ronald J. Fiskum,

(202) 586-9154; KSE, Inc. contact Dr. James R. Kittrell, (413) 549-5506

A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

In-Situ Electron Beam Processing for Radio Frequency Cavities - DOE contact Jerry Peters, (301) 903-5228; FM Technologies, Inc. contact Dr. Frederick M. Mako, (703) 425-5111

An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire - DOE contact Jerry Peters, (301) 903-5228; Alabama Cryogenic Engineering, Inc. contact Dr. John B. Hendricks, (256) 536-8629

High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling - DOE contact Jerry Peters, (301) 903-5228; EURUS Technologies, Inc. contact John Romans, (850) 574-1800

PHASE II (SECOND YEAR)

Thermally Stable Catalysts for Methane Combustion - DOE contact Richard A. Johnson, (304) 285-4564; TDA Research, Inc. contact Michael E. Karpuk, (303) 940-2301

Improved Precursors for Oxygen-Selective Membranes in Practical Devices for Methane Conversion - DOE contact Udaya Rao, (412) 386-4743; CeraMem Corporation contact Dr. Robert L. Goldsmith, (781) 899-4495

Supported Flat Plate Thin Films for Oxygen Separation - DOE contact Udaya Rao, (412) 386-4743; Eltron Research, Inc. contact Eileen E. Sammells, (303) 440-8008

A New Radiation Resistant Epoxy Resin System for Liquid Impregnation Fabrication of Composite Insulation - DOE contact Warren Marton, (301) 903-4958; Eltron Research, Inc. contact Eileen E. Sammells, (303)440-8008

Advanced Heat Sink Materials for Fusion Energy Devices - DOE contact Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. contact Timothy McKechnie, (256) 851-7653

Hybrid 3-D SiC/C High Thermal Conductivity Composites - DOE contact T. V. George, (301) 903-4957; MER Corporation contact R. O. Loutfy, (520) 574-1980

Co-Processed Ceramic Insulation for High Field Accelerator Magnets - DOE contact Jerry Peters, (301) 903-5228; Composite Technology Development, Inc. contact Dr. Naseem A. Munshi, (303) 664-0394

Improvement of High Field Performance and Reliability of Nb_3Sn Conductor by PIT Method - DOE contact Jerry Peters, (301) 903-5228; Supercon, Inc. contact Mrs. Elaine Tarkiainen, (508) 842-0174

Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings - DOE contact Yok Chen, (301) 903-3428; Spire Corporation contact Ronald S. Scharlack, (781) 275-7470

Large Area Filtered Arc Deposition of Carbon and Boron Based Hard Coatings - DOE contact Yok Chen, (301) 903-3428; UES, Inc. contact Francis F. Williams, Jr., (937) 426-6900

Meter Length YBCO Coated Conductor Development - DOE contact Yok Chen, (301) 903-3428; American Superconductor Corporation contact Dr. Tom Rosa, (508) 836-4200

Novel Catalyst for CH_4-CO Conversion - DOE contact Amy Manheim, (202) 586-1507; CeraMem Corporation contact Dr. Robert L. Goldsmith, (781) 899-4495

Flame Retardant Electrolytes for Li-Ion Batteries - DOE contact Susan Rogers, (202) 586-8997; EIC Laboratories contact Dr. A. C. Makrides, (781) 769-9450

Nonflammable Lithium-Ion Battery Electrolytes - DOE contact Susan Rogers, (202) 586-8997; TechDrive, Inc. contact Dr. Robert Filler, (630) 910-3729

INSTRUMENTATION AND FACILITIES

PHASE I

Development of a Universal Plastic Resin Composition Sensor for Whole Parts and Reground Mixtures - DOE contact Charlie Russomanno, (202) 586-7543; Spectracode, Inc. contact Dr. Edward Grant, (765) 494-9006

Sol-Gel Derived Neutron Detector Using a Lithiated Glass - DOE contact Helen Kerch, (301) 903-2346; Neutron Sciences, Inc. contact Andrew Stephan, (865) 523-0775

Development of an Ultra-Bright Electron Source for Scanning Transmission Electron Microscopy - DOE contact Dean Miller, (630) 252-4108; Nion Co. contact G. J. Corbin, (425) 576-9060

High Resolution Hybrid MCP Detector for Thermal Neutrons - DOE contact Helen Kerch, (301) 903-2346; Nova Scientific, Inc. contact Dr. Paul L. White, (508) 347-7679

Large Format MicroFiber Detector for Low Energy Neutrons - DOE contact Helen Kerch, (301) 903-2346; Nova Scientific, Inc. contact Dr. Paul L. White, (508) 347-7679

Pixel-Cell Neutron Detector and Read-Out System Meeting Requirements of Present and Future Neutron Scattering Facilities - DOE contact Helen Kerch, (301) 903-2346; Ordela, Inc. contact Daniel M. Kopp, (865) 483-8675

Novel Neutron Detector for High Rate Imaging Applications - DOE contact Helen Kerch, (301) 903-2346; Proportional Technologies, Inc. contact Dr. Jeffrey L. Lacy, (713) 747-7324

Smart Condition Monitor for High Temperature Turbine Blades - DOE contact Lane Wilson, (304) 285-1336; Advanced Fuel Research, Inc. contact Dr. Michael A. Serio, (860) 528-9806

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Advanced Membrane Technology for Biosolvents - DOE contact Charlie Russomanno, (202) 586-7543; Vertec Biosolvents LLC contact James E. Opre, (847) 803-0575

CO_2 Removal from Natural Gas - DOE contact Tony Zammerilli, (304) 285-4641; Carbozyme, Inc. contact Dr. Michael C. Trachtenberg, (732) 763-4809

PHASE II (SECOND YEAR)

Thin-Film Fiber Optic Sensors for Power Control and Fault Detection - DOE contact Alec Bulawka, (202) 586-5633; Airak Engineering, Inc. contact Paul Grems Duncan, (540) 864-6580

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Multiplexed Optical Fiber Chemical Sensor Arrays for Real-Time In Situ Monitoring of the Localized Corrosion Environment - DOE contact Kevin Zavadil, (505) 845-8442; Luna Innovations Incorporated contact Garrett S. Linkous, (540) 953-4274

Neutron Scattering Instrumentation for Measurement of Melt Structure - DOE contact Helen Kerch, (301) 903-2346; Containerless Research, Inc. contact John Nordine, (847) 467-2678

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Virtual-Impact Particle Sizing for Precursor Powders of Nb_3Sn and Bi-2212 Superconductors - DOE contact Jerry Peters, (301) 903-3233; Accelerator Technology Corporation contact Peter McIntyre, (979) 255-5531

Innovative Processing Methods for Superconducting Materials - DOE contact Jerry Peters, (301) 903-3233; Alabama Cryogenic Engineering, Inc. contact Mary T. Hendricks, (256) 536-8629

Oxide Dispersed Nanofluids for Next Generation Heat Transfer Fluids - DOE contact Glenn Strahs, (202) 586-2305; Nanopowder Enterprises, Inc. contact Dr. Gary S. Tompa, (732) 885-1088

Integrated Remanufacturing/Materials Recovery Process for Optimum Recycling of Plastics - DOE contact Charlie Russomanno, (202) 586-7543; Product Remanufacturing Centers Inc contact Arthur Krantz, (631) 424-2800

Plasma Spraying of $Nd_2Fe_{12}B$ Permanent Magnet Materials - DOE contact Sam Bader, (630) 252-4960; APS Material, Inc. contact Joseph Cheng, (937) 278-6547

OFFICE OF FUSION ENERGY SCIENCES

The mission of the Office of Fusion Energy Sciences (OFES) is to advance plasma science, fusion science, and fusion technology—the knowledge base needed for an economically and environmentally attractive fusion energy source. Fusion materials research is a key element of the longer-term OFES mission, focusing on the effects on materials properties and performance from exposure to the radiation, energetic particle, thermal, and chemical environments anticipated in the chambers of fusion experiments and energy systems.

The unique requirements on materials for fusion applications are dominated by the intense energetic neutron environment characteristic of the deuterium-tritium fusion reaction. Materials in the fusion chamber must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, "low activation" materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components).

Structural materials research focuses on issues of micro structural stability, fracture and deformation mechanics, and the evolution of physical and mechanical properties. This research provides a link between fusion and other materials science communities and contributes in niche areas toward grand challenges in general fields of materials science. Growth in the theory, modeling, and simulation elements of this research are providing for leveraging of advances in nanotechnology and computational materials science research.

Non-structural materials research focuses on plasma-facing materials that protect structural materials from intense heat and particle fluxes and extract surface heat deposited by plasmas without rapid deterioration and without emitting levels of impurities that could degrade plasma performance.

Fusion materials research is conducted with a high degree of international cooperation. Bilateral agreements with Japan enhance the ability of each party to mount fission reactor irradiation experiments. Agreements under the International Energy Agency provide for the exchange of information and the coordination of fusion materials programs in the U.S., Japan, Europe, Russia and China.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

231. **VANADIUM ALLOY AND INSULATING COATING RESEARCH**
$2,900,000
DOE contact: S. Berk (301) 903-4171
ORNL Contact S. Zinkle (865) 576-7220

Research is aimed at vanadium-based alloys for structural application in the chambers of fusion systems. The goals of the research, which focuses on the V-Cr-Ti system, are to identify promising candidate compositions, determine the properties of candidate alloys, and evaluate the response to irradiation conditions for anticipated fusion system operation. Critical issues include irradiation embrittlement (loss of fracture toughness), high-temperature creep, impurity corrosion, and joining. Compatibility studies are conducted between vanadium alloys and other candidate fusion materials, focusing on the effects of exposure to candidate coolants. Research is also conducted on electrically insulating coatings for elevated temperature environments. This work identifies promising candidate coating systems, develops coating technology, and conducts the experiments to demonstrate stability and self-repair needed for fusion applications. Work on vanadium alloys involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy, Coatings

232. **THEORY AND MODELING**
$700,000
DOE Contact: S. Berk (301) 903-4171
UCLA Contact: Nasr Ghoniem (310) 825-4866

Models and computer simulation, validated with experimental data, are combined to extend the understanding of the primary damage processes from irradiation effects. Research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that takes place in a material during neutron irradiation.. The goal is to establish models and methods that are able to extrapolate from the available data base to predict the behavior of structural components in fusion systems. Special attention is given to the energy range appropriate for the 14 MeV neutrons. Multiscale modeling applies results to evaluate the effects on properties of materials, especially the interactions of the irradiation produced defects with the flow dislocations during deformation processes. Investigations are conducted on (a) the limits of strength and toughness of materials based on dislocation propagation and interactions with crystalline matrix obstacles, (b) changes to thermal and electrical conductivity in materials based on electron and photon transport and scattering at the atomic level, (c) plastic instabilities and fracture processes in materials irradiated under projected fusion conditions, and (d) effects of the many materials, irradiation, and mechanical loading parameters on flow and fracture processes to establish understanding of controlling mechanisms. Techniques include atomistic computer simulation, atomic cluster modeling, Monte Carlo analysis, 3-D dislocation dynamics, and flow and fracture models. Research includes materials and conditions relevant to inertial fusion systems as well as magnetic systems.

Keywords: Modeling, Simulation, Irradiation Effects

233. **FERRITIC/MARTENSITIC STEEL RESEARCH**
$1,600,000
DOE Contact: S. Berk (301) 903-4171
ORNL Contacts: S. J. Zinkle (865) 576-7220

Research is aimed at iron-based alloys for structural application in the chambers of fusion systems. The goals of the research, which focuses on advanced ferritic/martensitic steel systems, are to identify promising candidate compositions, determine the properties of leading candidate alloys, and evaluate the response to irradiation conditions that simulate anticipated fusion system operation. Critical issues include irradiation embrittlement (focusing on DBTT transition shifts and loss of fracture toughness) and high temperature creep. Innovative nanocomposited steels are being explored for higher temperature applications than currently available ferritic steels. Work on this material class involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Steels, Irradiation Effects

234. **SiC/SiC COMPOSITES RESEARCH**
$1,400,000
DOE Contact: S. Berk (301) 903-4171
PNNL Contacts: R. J. Kurtz (509) 373-7515

Research is aimed at SiC/SiC composites for structural application in the chambers of fusion systems. This research is directed at furthering the understanding of the effects of irradiation on the SiC/SiC composite systems as the basis for developing superior composite materials for fusion structural applications. The focus of the work is on the evaluation of improved fibers and alternative interface layer materials. Critical issues include irradiation-induced reduction in thermal conductivity, leak-tightness, joining, and helium effects. Work on this material class involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Silicon Carbide, Composites, Irradiation Effects

235. **PLASMA FACING MATERIALS RESEARCH**
$2,000,000
DOE Contact: S. Berk, (301) 903-4171
SNL Contact: M. Ulrickson, (505) 845-3020

Plasma-facing materials must withstand high heat and particle fluxes from normal operation of fusion plasmas, survive intense surface energies from abnormal fusion plasma operation, such as plasma disruptions, withstand radiation damage by energetic neutrons, achieve sufficient lifetimes and reliability to minimise replacement frequency, and provide for reduced neutron activation to minimize decay heat and radioactive waste burdens. Research activities include improved techniques for joining beryllium or tungsten to copper alloys, development of joining techniques for refractory metals (e.g., W, Mo, Nb, V), development of enhancement schemes for helium cooling or liquid lithium cooling of refractory alloys, and thermal fatigue testing of tungsten and other refractory materials. The joining techniques being investigated include diffusion bonding, hot-isostatic pressing, furnace brazing and inertial welding. Tritium retention and permeation measurements are conducted in the Tritium Plasma Experiment and the PISCES plasma simulator facility. Refractory material work is centered on developing high temperature helium gas cooled or liquid metal cooled heat sinks for plasma facing components. The thermal fatigue testing and heat removal capability measurements are carried out on electron beam test systems.

Keywords: Plasma-Facing Materials, Refractory Metals

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 2001
OFFICE OF ENVIRONMENTAL MANAGEMENT - GRAND TOTAL	$3,042,996
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,042,996
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	366,666
Radiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere	200,000
Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes	173,333
Radiation Effects in Nuclear Waste Materials	313,333
New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization	300,000
Corrosion of Spent Nuclear Fuel: The Long-Term Assessment	148,333
Direct Investigations of the Immobilization of Radionuclides in the Alteration Products of Spent Nuclear Fuel	342,000
Decontamination of Radionuclides from Concrete During and After Thermal Treatment	0[1]
Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces	0[1]
Physical, Chemical and Structural Evolutioon of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	196,666
Mechanisms and Kinetics of Organic Aging in High-Level Nuclear Wastes	0[1]
Modeling of Spinel Settling in Waste Glass Melter	0[1]
Investigating Ultrasonic Diffraction Grating Spectroscopy and Reflection Techniques for Characterizing Slurry Properties	229,333
Chemistry of Actinides in Molten Glasses and its Correlation to Structural Performance of Solid Glasses: Filling the Knowledge Gap	213,333
Stability of High Level Radioactive Waste Forms	286,666
Physical Characterization of Solid-Liquid Slurries at High Weight Fractions Utilizing Optical and Ultrasonic Methods	273,333

[1]Prior Year Funding

OFFICE OF ENVIRONMENTAL MANAGEMENT

The Office of Environmental Management (EM) was established to effectively coordinate and manage the Department's activities to remediate the DOE Defense Complex and to properly manage waste generated by current operations. EM conducts materials research within two offices:

Office of Waste Management - The Office of Waste Management uses current technologies to minimize production of DOE-generated waste, alter current processes to reduce waste generation, and work with the Office of Science and Technology to develop innovative technologies for the treatment and disposal of present and future waste streams. The mission of the Office is to minimize, treat, store, and dispose of DOE waste to protect human health, safety, and the environment.

Office of Science and Technology - The Office of Science and Technology (OST) is responsible for managing and directing targeted basic research and focused, solution-oriented technology development programs to support the DOE Office of Environmental Management (EM). Programs involve research, development, demonstration, and deployment activities that are designed to produce innovative technologies and technology systems to meet national needs for regulatory compliance, lower life-cycle costs, and reduced risks to both people and the environment. Certain areas of the OST program focus on materials research in order to provide better, safer and less expensive approaches to identify, characterize and remediate DOE's waste problem.

Five Focus Areas have been formed to focus the EM-wide technology development activities on DOE's most pressing environmental management problems and are co-led by all EM offices:

Subsurface Contaminants. Hazardous and radioactive contaminants in soil and groundwater exist throughout the DOE complex, including radionuclides, heavy metals, and dense, nonaqueous phase liquids. Groundwater plumes have contaminated over 600 billion gallons of water and 50 million cubic meters of soil. In addition, the Subsurface Contaminants Focus Area is responsible for supplying technologies for the remediation of numerous landfills at DOE facilities. Technology developed within this speciality area provides effective methods to contain contaminant plumes and new or alternative technologies for remediating contaminated soils and groundwater.

Radioactive Tank Waste Remediation. Across the DOE Complex, hundreds of large storage tanks contain hundreds of thousands of cubic meters of high-level mixed waste. Primary areas of concern are deteriorating tank structures and consequent leakage of their contents. Research and technology development activities must focus on the development of safe, reliable, cost-effective methods of characterization, retrieval, treatment, and final disposal of the wastes.

Mixed Waste Characterization, Treatment, and Disposal. DOE faces major technical challenges in the management of low-level radioactive mixed waste. Several conflicting regulations together with a lack of definitive mixed waste treatment standards hamper mixed waste treatment and disposal. Disposal capacity for mixed waste is also expensive and severely limited. DOE now spends millions of dollars annually to store mixed waste because of the lack of accepted treatment technology and disposal capacity. In addition, currently available waste management practices require extensive, and hence costly waste characterization before disposal. Therefore, DOE must pursue technology that leads to better and less expensive characterization, retrieval, handling, treatment, and disposal of mixed waste.

Decontamination and Decommissioning. The aging of DOE's weapons facilities, along with the reduction in nuclear weapons production, has resulted in a need to transition, decommission, deactivate, and dispose of numerous facilities contaminated with radionuclides and hazardous materials. While building and scrap materials at the sites are a potential resource, with a significant economic value, current regulations lack clear release standards. This indirectly discourages the recovery, recycling, and/or reuse of these resources. The development of enhanced technologies for the decontamination of these materials, and effective communication of the low relative risks involved, will facilitate the recovery, recycle, and/or reuse of these resources. Improved materials removal, handling, and processing technologies will enhance worker safety and reduce cost.

Nuclear Materials. DOE is custodian for large quantities of fissile material and several thousand tons of spent nuclear fuels. Fissile materials were left in the manufacturing and processing facilities after weapons production was halted. These materials include plutonium solutions, plutonium metals and oxides, plutonium residues and compounds, highly enriched uranium, and other actinides. Research is needed to design processes for safe conversion of various types of fissile materials to optimal forms for safe storage, long-term storage, and ultimate disposition.
The projects listed in this report are managed under the Environmental Management Research Program (EMSP). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers,

provide opportunities for major cost reductions, reduce time required to achieve EM's mission goals, and, in general, address problems that are considered intractable without new knowledge. This program is designed to inspire breakthroughs in areas critical to the EM mission through basic research and is managed in partnership with ER. ER's well-established procedures are used for merit review of applications to the EMSP. Subsequent to the formal scientific merit review, applications that are judged scientifically meritorious are evaluated by DOE for relevance to the objectives of the EMSP. Since its inception in FY1996, the EMSP portfolio consists of 361awards amounting to a total of $300 million in three-year funding. Sixteen of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The FY 2001 component of materials research is estimated to amount to $3,042,996. The entire EMSP portfolio can be viewed on the World Wide Web at http://emsp.em.doe.gov/portfolio.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

236. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$366,666
DOE Contact: Justine Alchowiak (202) 586-4629
University of California at Los Angeles Contact: Robert F. Hicks (310) 206-6865
LANL Contact: Hans Herrmann (505) 665-6157

Decommissioning of transuranic waste (TRU) into low-level radioactive waste (LLW) represents the largest cleanup cost associated with the nuclear weapons complex. This project is developing a low-cost technology for converting TRU into LLW based on the selective plasma etching of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. However, this process is operated under vacuum, making it both expensive and difficult to apply to many nuclear wastes. A major breakthrough in this field was the demonstration of the operation of a g-mode, resonant-cavity, atmospheric-pressure plasma jet (APPJ). This jet etches kapton at between 10 and 15 m/hour, and tantalum at between 1 and 2 m/hour. Etching occurs below 373 K, so that delicate materials will not be destroyed by this process. The plasma jet may be used to selectively remove plutonium and other actinide elements by converting them into volatile compounds that are trapped by adsorption and filtration. Since the jet operates outside a chamber, many nuclear wastes may be treated, including machinery, duct-work, concrete and other building materials. At LANL, the source physics is being studied using Stark-broadening, microwave interferometry, and laser-induced fluorescence (LIF). The metastables, neutrals and radical species produced with mixtures of NF_3, CF_4, C_2F_6, O_2,He and Ar are being identified by LIF, optical emission spectroscopy (OES), laser Raman spectroscopy (LRS), coherent anti-Stokes Raman spectroscopy (CARS), and mass spectroscopy (MS). At UCLA, the elementary surface reactions of these species with tantalum and tungsten (surrogate metals for Pu) are being studied in ultrahigh vacuum using a supersonic molecular-beam coupled to the plasma jet. The surfaces are being characterized by X-ray photoemission (XPS), infrared spectroscopy (IR), low-energy electron diffraction (LEED), and scanning-tunneling microscopy (STM). In addition, plutonium etching experiments are being carried out at the Los Alamos Plutonium Facility. Recent improvements in the source design have made it compact, rugged, reliable and easily configured to treat objects of different sizes and shapes. The objectives of this research program are to fully characterize the discharge physics and chemistry, to engineer the exhaust containment system, and to test the plasma device on contaminated structures within the Department of Energy complex.

Keywords: Plasma Etching, Plutonium

237. **RADIATION EFFECTS ON SORPTION AND MOBILIZATION OF RADIONUCLIDES DURING TRANSPORT THROUGH THE GEOSPHERE**
$200,000
DOE Contact: Justine Alchowiak (202) 586-4629
University of Michigan Contacts: Lu-Min Wang, (313) 647-8530

Site restoration activities at DOE facilities and the permanent disposal of nuclear waste inevitably involve understanding the behavior of materials in a radiation field. Radionuclide decay and associated radiation effects lead to physical and chemical changes in important properties (e.g., sorption and cation exchange capacity). During the past three years, radiation effects in selected near-field materials have been evaluated in accelerated laboratory experiments utilizing energetic electrons and ions and *in situ* transmission electron microscopy (TEM). Zeolites and layered silicates were found to be highly susceptible to irradiation-induced solid-state amorphization. The critical doses for complete amorphization of these phases are as low as <0.1 displacement per atom (dpa) or 108 GY in ionization energy deposition (i.e., the dose for a zeolite with 10 wt.% loading of ^{137}Cs in 400 years). Even partial amorphization will cause a dramatic reduction (up to 95%) in ion-exchange and sorption/desorption capacities for radionuclides, such as Cs and Sr. Because the near-field or chemical processing materials, e.g., zeolites or crystalline silicotitanate (CST), will receive a substantial radiation dose after they have incorporated radionuclides, the results suggest that radiation may, in some cases, retard the release of sorbed or ion-exchanged radionuclides. These results have a direct bearing on repository performance assessments (e.g., the extent to which zeolites can retard the release of radionuclides) and on the technologies used to process high-level liquid waste (e.g., separation of ^{137}Cs from HLW using CST at the Savannah River Site).

Radionuclides to be studied include Cs, Sr, U, and Se, which are important because: 1)they represent a range of sorptive behavior that should bracket the behavior of most other radionuclides (except ^{99}Tc) and 2) they are considered to make important contributions to total radiation exposures, as illustrated in the recent Total Systems Performance Assessment-Viability Assessment of the proposed repository at Yucca Mountain. Selected clay and zeolite samples will be irradiated with high energy electrons, high energy ions and neutrons to simulate the radiation effects from a variety of radioactive decay processes at a much accelerated rate using a unique combination of irradiation facilities available at the University of Michigan (the Ford Nuclear Reactor and the Michigan Ion Beam Laboratory). Ion exchange/sorption experiments will be conducted on samples irradiated to various doses to determine the impact of the radiation effects on the sorption capacity and retention of radionuclides. Novel ion implantation and surface analysis techniques, e.g., atomic force microscopy and Z-contrast high resolution scanning transmission electron microscopy (STEM), will be used to identify atomic-scale effects of radiation damage associated with single or small clusters of radionuclides sorbed onto mineral surfaces.

Keywords: Radiation Effects, Near-Field, Geologic Repository

238. **IRON PHOSPHATE GLASSES: AN ALTERNATIVE FOR VITRIFYING CERTAIN NUCLEAR WASTES**
$173,333
DOE Contact: Justine Alchowiak (202) 586-4629
University of Missouri-Rolla Contact:
Delbert E. Day (573) 341-4354

Borosilicate glass is the only material currently approved and being used to vitrify high level nuclear waste. Unfortunately, many high level nuclear waste feeds in the U.S. contain components which are chemically incompatible with borosilicate glasses. Current plans call for vitrifying even these problematic waste feeds in borosilicate glasses after the original waste feed has been pre-processed and/or diluted to compensate for the incompatibility. However, these pre-treatment processes, as well as the larger waste volumes resulting from dilution, will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

A low cost and technically effective alternative waste form based on a new family of iron-phosphate glasses which appear to be well suited for many waste feeds, especially those which are incompatible with borosilicate glasses, has recently been developed. However, the scientific and technical knowledge base that is needed to vitrify nuclear waste in iron phosphate glasses on a production scale is currently lacking. In addition, the high priority wastes that are likely to cause problems in borosilicate melts need to be identified and property data need to be acquired for iron phosphate wasteforms made from these wastes. This research is addressing these needs, using techniques such as EXAFS, XANES, XPS, X-ray and neutron diffraction, IR, SEM, Mössbauer spectroscopy and DTA/DSC to obtain the information needed to demonstrate that iron phosphate glasses can be used to vitrify those nuclear wastes which are poorly suted for borosilicate glasses.

Keywords: Iron Phosphate Glasses, Vitrification, Nuclear Waste

239. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$313,333
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The objective of this project is to develop a fundamental understanding of radiation effects in glass and ceramics, as well as the influence of radiation effects on aqueous dissolution kinetics. This study will provide the underpinning science to develop improved glass and ceramic waste forms for the immobilization and disposition of high-level tank waste, excess plutonium, plutonium residues and scrap, surplus weapons plutonium, other actinides, and other nuclear waste streams. Furthermore, this study will develop predictive models for the performance of nuclear waste forms and stabilized nuclear materials. The research focuses on the effects of alpha and beta decay on defect production, defect interactions, diffusion, solid-state phase transformations, and gas accumulation, and dissolution kinetics. Plutonium incorporation, gamma irradiation, ion-beam irradiation, and electron beam irradiation are used to simulate the effects of alpha decay and beta decay on relevant glasses and ceramics in experimental studies. Computer simulation methods are used to provide an atomic-level interpretation of experimental data, calculate important fundamental parameters, and provide multi-scale computational capabilities over different length (atomic to macroscopic) and time (picoseconds to millenia) scales.

Keywords: Glass, Ceramics, Radiation Effects

240. **NEW METAL NIOBATE AND SILICOTITANATE ION EXCHANGERS: DEVELOPMENT AND CHARACTERIZATION**
$300,000
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Previous research by this group provided preliminary data of a novel class of niobate-based molecular sieves (Na/Nb/M/O, M=transition metals) that show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations) and novel silicotitanate phases that are also selective for divalent cations. Furthermore, these materials are easily converted by a high-temperature *in situ* heat treatment into a refractory ceramic waste form with low cation leachability. The new niobate-based waste form is a perovskite phase, which is also a major component of Synroc, a titanate ceramic waste form used for sequestration of high-level wastes (HLW) from reprocessed, spent nuclear fuel. These new niobate ion exchangers also showed orders of magnitude better selectivity for Sr^{2+} under acid conditions than any other material.

The goal of this project is to provide DOE with alternative materials that can exceed the performance of monosodium titanate (MST) for strontium and actinide removal at the Savannah River Site (SRS), remove strontium from acidic waste at Idaho National Engineering and Environmental Laboratory (INEEL), and sequester divalent cations from contaminated groundwater and soil plume. The research team will focus on three tasks that will provide both the basic research necessary for the development of highly selective ion exchange materials and also materials for short-term deployment within the DOE complex: 1) structure/property relationships of a novel class of niobate based molecular sieves (Na/Nb/M/O, M=transition metals), which show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations); 2) the role of ion exchanger structure change (both niobates and silicotitanates) on the exchange capacity (for elements such as strontium and actinide-surrogates), whichresult from exposure to DOE complex waste simulants; 3) thermodynamic stability of metal niobates and silicotitanate ionexchangers.

Keywords: Niobate, Silicotitanate, Ion Exchanger

241. **CORROSION OF SPENT NUCLEAR FUEL: THE LONG-TERM ASSESSMENT**
$148,333
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Spent nuclear fuel accounts for over 95% of the total radioactivity in the radioactive wastes in the United States that require disposal, disposition, or remediation. The UO_2 in spent nuclear fuel is not stable under oxidizing conditions. Under oxidizing conditions, the U(IV) has a strong tendency to exist as U(VI) in the uranyl molecule, UO_2^{2+}. The uranyl ions react with a wide variety of inorganic and organic anions to form complexes which are often highly soluble. The result is rather rapid dissolution of UO_2 and the formation of a wide variety of uranyl oxide hydrates, uranyl silicates and uranyl phosphates. The kinetics for this transformation are rapid, essentially instantaneous on geologic time scales. Under reducing conditions, UO_2 is stable, but may alter to U^{4+} compounds such as coffinite, $USiO_4$, depending on groundwater compositions. Under both oxidizing and reducing conditions, the formation of new uranium phases may lead to the release or retardation of trace elements, such as the fission product elements and actinides in spent nuclear fuel. Over the long term, and depending on the extent to which the secondary uranium phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous experimental studies and field studies have established that natural uranite and its alteration products are good "natural analogues" for studying the corrosion of UO_2 in spent nuclear fuel. This research program is addressing the following issues:

- What are the long-term corrosion products of natural UO_{2+x}, uraninite, under oxidizing and reducing conditions?
- What is the paragenesis or the reaction path of the phases that form during alteration? How is the sequence formation related to the structure of these uranium phases and reacting groundwater composition?
- What is the trace element content in the corrosion products as compared to the original UO_{2+x}? Do the trace element contents substantiate models developed to predict radionuclide incorporation into the secondary phases?
- Are the corrosion products accurately predicted from geochemical codes (e.g., EQ3/6) that are used in performance assessments?

- How persistent over time are the metastable phase assemblages that form? Will these phases serve as effective barriers to radionuclide release?

Experimental results and theoretical models for the corrosion of spent nuclear fuel under oxidizing and reducing conditions will be tested by comparison to results from studies of samples from the Oklo natural fission reactors.

Keywords: Uranium Oxides, Minerology, Corrosion, Phase Stability

242. **DIRECT INVESTIGATIONS OF THE IMMOBILIZATION OF RADIONUCLIDES IN THE ALTERATION PRODUCTS OF SPENT NUCLEAR FUEL**
$342,000
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This project emphasizes the synthesis of uranium phases and uranium phases doped with certain radionuclides in order to examine radionuclide incorporation in uranyl compounds. The identities of alteration phases important for spent-fuel corrosion will be gleaned from the results of long-term experiments on the corrosion of spent UO_2 fuel and unirradiated UO_2, as well as more recent studies of U-metal fuel corrosion, that are currently underway at ANL. The focus will be on synthesizing actinide compounds similar to those that have been identified as corrosion products of spent uranium-based fuels. The goals of the experiments are to synthesize and characterize actinide and fission-product host phases formed on U-based waste forms under oxidizing conditions, such as expected at the candidate geological repository at Yucca Mountain. Target phases for synthesis include those identified in current corrosion experiments with U-based fuels being conducted at Argonne. Those experiments demonstrate that many radionuclides are retained in U-bearing alteration products. Synthesis and characterization of U(VI) phases doped with specific radionuclides helps clarify the mechanisms of radionuclide incorporation into uranyl-based compounds. Where possible, stable-isotope equivalents of radionuclides are used during synthesis; however, pure Np and Pu analogues of selected uranium compounds will also be synthesized. In addition, U compounds doped with low levels of selected radionuclides will be characterized in order to understand mechanisms of trace-element substitution.
Methods used to characterize solid phases include X-ray powder diffraction and transmission electron microscopy. Selected samples are also analyzed by single-crystal X-ray structure analyses and X-ray absorption spectroscopy, where possible.

Keywords: Uranium Oxides, Minerology, Phase Stability, Corrosion, Radionuclides

243. **DECONTAMINATION OF RADIONUCLIDES FROM CONCRETE DURING AND AFTER THERMAL TREATMENT**
$0[1]
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The total area of contaminated concrete within all DOE facilities is estimated at 7.9 x $10^8 ft^2$ or approximately 18,000 acres with the major contaminating radionuclides being U, ^{90}SR, ^{60}Co, and ^{137}Cs (Dickerson et. al. 1995). Techniques to decontaminate concrete through the application of heat (including microwaves, infrared radiation, lasers, plasma torch, etc.) have centered on the generally known deterioration of concrete strength with imposed thermal stress. These strategies have all attempted to spall or scabble contaminated solids from the concrete surface and to maximize the particular technology's capability to that end. However, in addition to the imprecisely defined knowledge of the physical effects of specific heat treatments on concrete (final temperature, heating rate, and type of concrete aggregate), concomitant behavior of DOE's major radioactive contaminants (^{137}Cs, U, ^{90}Sr, and ^{60}Co) during thermal treatment is very poorly known. This research will determine the thermal effects between 100 and 1400 C on concrete engineering properties (compressive strength, strain, porosity, bulk density, and cracking), chemical properties (dehydration, mineral phase change, and solubility), and contaminant behavior as a function of final temperature, heating rate, and aggregate type (none, limestone, or silica); thermal effects on contaminants and concrete are depicted conceptually in Figure 1. Major effects on radionuclide transport via direct volatilization (particularly for ^{137}Cs and ^{60}Co) during heating are anticipated to lead to *in situ* decontamination techniques. Changes in the extractability of radionuclides from heat affected concrete will be measured, using short-lived radioisotopes, to ascertain changes in decontamination potential following thermal treatment. Detailed finite-element modeling of heat flow in concrete and resulting mechanical stresses (from pore pressure and thermal expansion) of optimal thermal treatments will be completed so that effects on laboratory-sized specimens can be extrapolated to field-scale thermal treatments on concrete mechanical properties and contaminant behavior. Expected results will be a thorough and detailed

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understanding of the thermal effects on concrete engineering properties and concomitant radionuclide behavior including a detailed empirical data base. Specific decontamination technologies using thermal stressing of concrete will then be able to predict their effects rather than continue with DOE's apparent present approach of supporting novel thermal technologies without either a basic understanding of the limits of thermal effects on concrete or the fate and behavior of key radionuclides.

Keywords: Concrete, Radionuclides, Decontamination

244. **MECHANISMS OF RADIONUCLIDE-HYDROXYCARBOXYLIC ACID INTERACTIONS FOR DECONTAMINATION OF METALLIC SURFACES**
$0[1]
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State University of New York at Stony Brook
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This project addresses key fundamental issues involved in the use of simple and safe methods for the removal of radioactive contaminants from slightly contaminated steel and other surfaces at the DOE sites so that the metals can be reused. The objectives are to (i) determine the nature of the association of radionuclides U, Pu, Co and Sr with stainless steel, and (ii) selectively remove the radionuclides using hydroxycarboxylic acids (citric acid and its analogs). The basic mechanisms involving coordination, complexation, dissolution and removal will be elucidated in a systematic manner.

This is a collaborative research project between Brookhaven National Laboratory (BNL) and the State University of New York at Stony Brook (SUNY-SB). This project is divided into three phases. In Phase I the basic mechanism of interaction of actinides with metal oxides on metallic surfaces will be investigated. Phase II will determine the interaction of hydroxycarboxylic acids citric, malic and tartaric acids with the actinide contaminated metallic surfaces. Phase III involves investigation of interaction of hydroxycarboxylic acid with actual contaminated samples from DOE sites and interpretation of results based on knowledge gained from Phases I and II. The nature of radionuclide association with representative metal oxides typically formed on metallic surfaces which have undergone oxidation characteristic of long term environmental exposure will be investigated. The rate and extent of incorporation of radionuclide into amorphous and crystalline forms of iron oxides (goethite, hematite, magnetite and lepidocrocite), and metallic coupons will be determined. Exposure of metallic coupons to radionuclides during and following accelerated aqueous corrosion will utilize standard electrochemical cells and equipment. Advanced spectroscopic techniques (XPS, XANES, EXAFS, EDX, SIMS, FTIR and LD-ITMS at PNNL) will be used to characterize the (1) nature of the radionuclide association with the metal oxides and contaminated surfaces, and (2) radionuclide-citrate complexes and mixed-metal (actinide-metal-citrate) complexes that have been removed from contaminated surfaces. In addition, the photochemical and biochemical degradation of the resulting actinide-organic complexes will be examined, with application to recovery of radionuclides in a concentrated form and reduction of secondary waste generation.

Keywords: Radionuclides, Decontamination, Actinides, Corrosion

245. **PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW**
$196,666
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Natural and synthetic zeolites are extremely versatile materials. They can adsorb a variety of liquids and gases, and also take part in cation exchange reactions. Zeolites are easy to make, they can be synthesized from a wide variety of natural and man made materials. One such combination is metakaolinite and sodium hydroxide solution. The objective of this research is to adapt this well known reaction for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites.

It has been established that a mixture of calcined equivalent ICPP waste (sodium aluminate/hydroxide solution containing 3:1 Na:Al) and fly ash and/or metakaolinite can be cured at various temperatures to produce a monolith containing Zeolite A (80 C) or Na-P1 plus hydroxysodalite (130 C) dispersed in an alkali aluminosilicate hydrate matrix. The zeolitization process is a simple one and as such could be a viable alternative for fixation of low activity waste (LAW) salts and calcines. Dissolution tests have shown these materials to have superior retention for alkali, alkaline earth and heavy metal ions.

The technology for synthesizing zeolites is well documented for pure starting materials, but relatively little is known about the process if metakaolinite is mixed with a complex mixture of oxides containing nearly every element in the periodic table. The purpose of the

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proposed work is to develop a clearer understanding of the advantages and limitations of producing a zeolite-containing waste form from calcined radioactive waste, i.e. the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on their performance. To accomplish this, two waste forms representative of solutions in storage at the Hanford and Savannah River sites will be simulated. Because nitrate is detrimental to the process, the LAW will be calcined at various temperatures (w/wo sugar) to maximize the reactivity of the resultant mix of oxide phases while minimizing the loss of volatiles. The oxides will be mixed with varying amounts and types of metakaolinite, small amounts of other chemicals (alkali hydroxides and/or carbonates, zeolite seeds, templating agents) and enough water to make a paste. The paste will then be cured (in-can) at a variety of temperatures (80 -100 C). Once reaction rates for the process are established, MAS NMR and TEM will be used to study the atomic-level structure of the solids. X-ray diffraction will be used to examine the degree of crystallinity of the waste forms. An environmental SEM will be used to track the development of microstructure in real time. An electron microprobe will be used to analyze the phases in the waste form. Attempts will be made to relate changes in phase chemistry and microstructure to distribution coefficients and dissolution data. Compressive and bending strength tests will be used to determine mechanical behavior and standard leach tests will be used to determine the potential consequences of cation exchange reactions. Since simulated waste is not an adequate predictor, a major portion of the proposed work will be carried out at the Savannah River Technology Center, using actual LAW samples obtained from the Savannah River site.

Keywords: Zeolites, Radioactive Waste

246. **MECHANISMS AND KINETICS OF ORGANIC AGING IN HIGH-LEVEL NUCLEAR WASTES**
$0[1]
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Highly radioactive wastes stored at Hanford and Savannah River DOE sites have unresolved questions relating to safety of the stored waste, as well as needs for safe, effective, and efficient waste processing to minimize the volume of high-level waste (HLW) streams for disposal. HLW undergoes constant irradiation from decaying radionuclides resulting in an array of radiation and thermochemical effects that directly impact issues concerning storage, retrieval, and pretreatment of the wastes. Heat from nuclear decay and from chemical processing (e.g., evaporation campaigns and tank transfers) drive thermal reactions of waste constituents, especially organic complexants. Radiolytic and thermochemical processes have been shown to degrade ("age") organic solutes into smaller fragments of lower energy content, reducing hazards associated with deflagration of nitrate organic mixtures while contributing to hazards such as the generation of toxic, flammable and potentially explosive gases (i.e., volatile organics, NH_3, H_2, and N_2O).

The goal of this project is to develop a fundamental understanding of organic aging and to assemble a model which describes and predicts the thermal and radiolytic aging of organic compounds in high level wastes. Kinetics will be measured and products and mechanisms of organic reactions occurring under conditions of waste storage, retrieval, and processing will be elucidated. Much emphasis will be placed on studying thermal effects, since organic reaction mechanisms and effects of varying conditions are uncertain. Organic complexants are of greatest concern regarding both safety and pretreatment since they have been found to degrade to gases, combust in dry wastes, and interfere with radionuclide separations. Therefore, efforts will focus on studying the reactions of these organic chemicals and associated degradation products.

Keywords: Oxidation, Organics, Radionuclides, Aging

247. **MODELING OF SPINEL SETTLING IN WASTE GLASS MELTER**
$0[1]
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The topic of this multi-institutional bi-national research is the formation and settling of spinel, the most common crystalline phase that precipitates in molten high-level waste (HLW) glass. For the majority of HLW streams, spinel formation in the HLW melter limits the waste fraction in glass because accumulation of spinel interferes with melter operation and shortens its lifetime. Hence, understanding spinel formation and behavior is important for HLW vitrification technology and economy, which call for the highest waste loading that is compatible with the quality and processability of the waste form.

Spinel is a product of an interaction between Cr_2O_3, Fe_2O_3, NiO, FeO, and other oxides, which are components of virtually all HLW streams at Hanford and Savannah River. Understanding and modeling the kinetics of spinel formation and the dynamics of spinel behavior in a waste glass melter will result in a reliable

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prediction and control of the rate of spinel settling and accumulation. The spinel settling rate will be predicted by mathematical modeling for which reliable experimental values of coefficients and material parameters will be obtained by laboratory studies. This approach combines the materials science, hydrodynamics, and mathematical modeling of spinel behavior in HLW glass melters.

Keywords: Spinel Formation, Equilibria, High-Level Waste Glass

248. **INVESTIGATING ULTRASONIC DIFFRACTION GRATING SPECTROSCOPY AND REFLECTION TECHNIQUES FOR CHARACTERIZING SLURRY PROPERTIES**

$229,333
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The U.S. Department of Energy (DOE) has millions of gallons of radioactive liquid and sludge wastes that must be retrieved from underground storage tanks. This waste, in the form of slurries, must be transferred and processed to a final form, such as glass logs. On-line instrumentation to measure the properties of these slurries in real-time during transport is needed in order to prevent plugging and reduce excessive dilution. This project is a collaborative effort between Pacific Northwest National Laboratory (PNNL) and the University of Washington to develop a completely new method for using ultrasonics to measure the particle size and viscosity of a slurry. The concepts are based on work in optics on grating-light-reflection spectroscopy (GLRS) at the University of Washington and some preliminary work on ultrasonic diffraction grating spectroscopy (UDGS) that has already been carried out at PNNL. The project objective is to extend the GLRS theory for optics to ultrasonics, and to demonstrate its capabilities of UDGS. The viscosity of a slurry is measured by using the multiple reflections of a shear wave at the slurry-solid interface. This new ultrasonic method could result in an instrument that would be simple, rugged, and very small, allowing it to be implemented as part of a pipeline wall at facilities across the DOE complex.

Keywords: Diffraction Grating, Spectroscopy, Ultrasonic, Slurry, Viscosity, Particle Size

249. **CHEMISTRY OF ACTINIDES IN MOLTEN GLASSES AND ITS CORRELATION TO STRUCTURAL PERFORMANCE OF SOLID GLASSES: FILLING THE KNOWLEDGE GAP**

$213,333
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Chemical processes occurring in molten glasses are key elements in determining efficient immobilization and the long term stability of glasses. The underlying goal of this research is to make use of high-temperature spectroscopic techniques to increase our fundamental understanding of the vitrification process, specifically the relationship between the chemistry of molten glasses and the structural features of final solid glasses. The fundamental knowledge gained in this study will fill a crucial knowledge gap concerning chemistry of actinides in molten glasses and have a broad impact on the design and construction of advanced vitrification processes. High temperature UV/Visible and near-IR spectral data will be used to investigate the solubility of actinide species in various molten glasses as a function of the composition and temperature. These data will be used to develop a new “optical basicity” scale for actinide stability and speciation in oxide glasses in analogy to the common pH scale used to define the acid-base properties of aqueous systems. Fluorescence lifetime distribution methods, fluorescence line-narrowing spectroscopy and X-ray absorption spectroscopy (XAS) will provide information on the local environment of the actinides while EPR and x-ray absorption edge positions will be used to define the oxidation states of actinide species in glasses. The combination of the optical basicity scale and structural information from fluorescence and XAS investigations, will be used to produce a detailed description of the identities and behavior of actinide species in silicate-based glasses. This stability model will be correlated to actinide leaching behavior for a glass matrix and offers a simple but powerful set of spectral “fingerprints” to predict the behavior of actinide species when immobilized in a glass.

Keywords: Molten Glasses, Spectroscopy, X-Ray Absorption, Actinides

250. **STABILITY OF HIGH LEVEL RADIOACTIVE WASTE FORMS**
$286,666
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High-level waste (HLW) glass compositions, processing schemes, limits on waste loading, and corrosion/ dissolution release models are dependent on an accurate knowledge of liquidus temperatures and thermochemical values. Unfortunately, existing models for the liquidus are empirically-based, depending on extrapolations of experimental information. In addition, present models of leaching behavior of glass waste forms use simplistic assumptions of the thermochemistry or experimentally measured values obtained under non-realistic conditions. There is thus a critical need for both more accurate and more widely applicable models for HLW glass behavior. In a previous project significant progress was made in modeling HLW glass. Borosilicate glass was accurately represented along with the additional FeO-Fe_2O_3, Li_2O, K_2O, MgO, and CaO components. Nepheline precipitation, an issue in Hanford HLW formulations, was modeled and shown to be predictive. The objective of this effort is to continue the development of a basic understanding of the phase equilibria and solid solution of HLW glasses, incorporating other critical waste constituents including, S, Cr, F, P, actinides and rare earths. With regard to a fundamental understanding of solution oxides, there should be added insights on defect chemistry, interstitial behavior, clustering, and the energetics of metal oxide solutes.

Keywords: High-level waste, Glass, Phase equilibria

251. **PHYSICAL CHARACTERIZATION OF SOLID-LIQUID SLURRIES AT HIGH WEIGHT FRACTIONS UTILIZING OPTICAL AND ULTRASONIC METHODS**
$273,333
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Liquid sodium-bearing waste (SBW) can be calcined and solidified using metakaolinite and a limited amount of water. The processing does not require expensive specialized equipment or exotic materials but rather it can be done using conventional cement and/or concrete mixing equipment. The final product is cured at relatively low temperatures producing a dense ceramic-like material (hydroceramic) with strength in the 300-400 psi range and leach rates comparable to glass waste forms with similar waste loading. This product is stable in realistic geologic settings due to the *in situ* growth of zeolites. Data from a previous project have shown that hydroceramics could well be a viable alternative for fixation of low activity sodium-bearing waste. The objective of this continuation study is to further adapt this technology for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites. This work is aimed at developing a clearer understanding of the advantages and limitations of producing a zeolite-containing hydroceramic from the low activity SBW at these sites, i.e., the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on the performance of the waste form. In addition, the processing method will be further refined to increase waste loading in the hydroceramics, with the objective of making the calcine fit the zeolitization process as well as possible. It is anticipated that by tailoring the calcination process, it will be possible to encapsulate many more radionuclides without sacrificing the performance of the waste form, thereby creating a better hydroceramic waste form.

Keywords: Hydroceramic, Zeolites, Sodium-Bearing Waste, Calcination

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 2001
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY - GRAND TOTAL	$15,454,365
OFFICE OF SPACE AND DEFENSE POWER SYSTEM	$4,498,000
SPACE AND NATIONAL SECURITY PROGRAMS	$4,498,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$3,698,000
Maintain the Capabilities and Facilities to Produce DOP-26 Iridium Alloy Blank and Foil Stock Material, Manufacture Clad Vent Sets, and Manage the Iridium Inventory	1,988,000
Carbon-Bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	330,000
Alloy Development Characterization, Mechanical Property Testing, and Insulation Outgassing Assessment for Space and Advanced Terrestrial Systems	980,000
New Methods for Joining Beta“-Alumina to Niobium 1% Zirconium for Alkali Metal to Thermal Electric Converters (AMTEC)	100,000
AMTEC Electrode and Beta”-Alumina Solid Electrolyte Development	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$800,000
Fabrication Development and Materials Production for AMTEC Converters	800,000
OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION	$10,956,365
NUCLEAR ENERGY PLANT OPTIMIZATION	$3,189,370
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,189,370
Steam Generator NDE Test Mockup Facility	350,000
Advanced Eddy-Current Inspection System for Detection and Characterization of Defects in Steam Generator Tubes	300,000
Develop Empirical Data to Characterize Aging Degradation of Polymers Used in Electrical Cable	327,000
Develop Condition Monitoring (CM) Techniques for Electrical Cable	591,019
Mechanical Behavior of Irradiated Structural Stainless Steels	407,000
Fatigue Management	560, 638
Assessment of Aging Effects on Components and Structures from Nuclear Power Plants	50,000
Irradiation-Induced Swelling and Stress Relaxation of PWR Reactor Core Internal Components	603,713

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY (continued)

	FY 2001
OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION (continued)	
NUCLEAR ENERGY RESEARCH INITIATIVE	$7,766,995
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$3,901,999
Novel Concepts for Damage-Resistant Alloy in Next Generation Nuclear Power Systems	560,000
Advanced Ceramic Composites for High-Temperature Fission Reactors	260,000
Development of Improved Burnable Poisons for Commercial Nuclear Power Reactors	415,000
Fuel for a Once-Through Cycle (Th, U) O_2 in a Metal Matrix	360,035
Advanced Proliferation Resistant, Lower Cost, Uranium-Thorium Dioxide Fuels for Light Water Reactors	1,132,742
Development of a Stabilized Light Water Reactor (LWR) Fuel Matrix for Extended Burnup	360,348
An Innovative Ceramic Corrosion Protection System for Zircaloy Clading	228,874
A Single Material Approach to Reducing Nuclear Waste Volume	210,000
Developing Improved Reactor Structural Materials Using Proton Irradiation a Rapid Analysis Tool	375,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,864,996
Application of Innovative Experimental and Numerical Techniques for the Assessment of Reactor Pressure Vessel Structural Integrity	70,000
Innovative Chemithermal Techniques for Verifying Hydrocarbon Integrity in Nuclear Safety Materials	354,067
Continuous-Wave Radar to Detect Defects within Heat Exchanger & Steam Generator Tubes	372,000
Fundamental Mechanisms of Corrosion of Advanced Zirconium Based Alloys at High Burn-Up	690,777
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OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF SPACE AND DEFENSE POWER SYSTEMS

SPACE AND NATIONAL SECURITY PROGRAMS

Space and National Security Programs include the development and production of radioisotope power systems (RPS) for both space and terrestrial applications and provide the technical direction, planning, demonstration and delivery of space nuclear reactor power and propulsion systems. During FY-2001, materials programs included: 1) maintaining iridium alloy Blank and Foil and Clad Vent Sets (CVS) production capabilities and facilities by manufacturing flight quality CVSs and installing integral weld shields in existing hardware, 2) documenting CBCF production techniques by video and approving a new procedure for sulfur analysis of the material, 3) production of vacuum-arc cast Mo-41%Re stock material and fabrication development and construction of AMTEC converters and 4) providing materials characterization data and properties of materials (DOP-26, DOP-40, Haynes 25, Mo-41%Re) used in space power and terrestrial RPS applications.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

252. **MAINTAIN THE CAPABILITIES AND FACILITIES TO PRODUCE DOP-26 IRIDIUM ALLOY BLANK AND FOIL STOCK MATERIAL, MANUFACTURE CLAD VENT SETS, AND MANAGE THE IRIDIUM INVENTORY**
$1,988,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
ORNL Contacts: J. P. Moore (865) 574-8258 and E. K. Ohriner (865) 574-8519

Iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al additions) is the fuel clad capsule material for isotope heat sources employed in space power systems for NASA deep space missions. The production capabilities and facilities for producing the Blank and Foil stock material at ORNL are maintained by continuing all production activities (powder processing, melting, extrusion, rolling, etc.) at a reduced level to supply limited quantities of blank and foil for CVS production maintenance activities. The CVS production activity produces flight quality clad sets for inventory and maintains the production capabilities and facilities for future production campaigns. The iridium inventory for DOE is maintained, audited, and reported annually.

In FY-2001 an iridium ingot was extruded and 30 flight quality blanks were produced and stored. The qualification of a commercial vendor for glow discharge mass spectrometry determination of elemental composition of iridium alloys was initiated and progress toward the qualification reported. The CVS production task shipped 66 modified shield cup assemblies with the integral weld shields to Los Alamos National Laboratory (LANL). Nine flight quality Clad Vent Sets from Qualification Production at ORNL were also shipped to LANL. An additional five clad vent sets were produced.

Keywords: Iridium Processing, Melting, Extrusion, Clad Vent Sets

253. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION**
$330,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
ORNL Contact: G. Romanoski (865) 574-4838

Carbon-bonded carbon fiber (CBCF) type thermal insulation is employed in isotopic General Purpose Heat Source (GPHS) Module assemblies for use in current GPHS-RTGs (radioisotope thermoelectric generator). This material was originally employed in GPHS-RTGs for Galileo/NASA (1989 launch) and Ulysses/NASA-ESA (1990 launch) Missions. Material produced for the Cassini Mission (1997 launch) was made with a replacement carbon fiber utilizing an optimized process and process controls. In FY-2001 a draft video was made which documents all production and qualification tasks. This video will be used as a training tool and record of production details. Also, a revised procedure was developed and approved for determination of sulfur in graphite and carbon by a LECO Analyzer.

Key words: Insulator/Thermal, High Temperature Service, Fibers

254. **ALLOY DEVELOPMENT CHARACTERIZATION, MECHANICAL PROPERTY TESTING, AND INSULATION OUTGASSING ASSESSMENT FOR SPACE AND ADVANCED TERRESTRIAL SYSTEMS**
$980,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
ORNL Contacts: E. P. George (865) 574-5085, J. P. Moore (865) 574-8258 and R. W. Swindeman (865) 574-5108

The technology tasks provide the materials characterization, mechanical property information, and assessment of material behavior in specific applications to support various RPS program needs. The characterization of iridium alloy DOP-26 has identified the effect of various impurities and the effect on manufacturing and service reliability. An alternate iridium alloy (DOP-40) containing less thorium and the addition of cerium has been developed and shown to have desirable properties. Mechanical property determinations are made on various alloys after thermal aging to assess their suitability for long-term terrestrial and deep space exploratory missions. Assessments are made of internal component materials for milliwatt generator outgassing characteristics.

Accomplishments were made in several areas during FY2001. Oxidation compatibility testing was conducted on the DOP-40 iridium alloy and strain effects from bending, rolling, and forming were assessed for the DOP-26 alloy. Thermal aging studies are being conducted on Mo-41%Re and the effect of grain size on aging of Haynes 25 was conducted. The tensile measurements of unaged base metal and weldment specimens of Haynes 25 were completed along with 6000 h aged base metal specimens. The pressure burst test facilities and procedures for testing Advanced Long-Term Battery (ALTB) Haynes 25 capsules were completed. Outgassing characteristics of milliwatt generator insulation material were measured to assess the performance of the generator over the expected service life.

Keywords: Iridium Alloys, Haynes 25, Material Characterization, Thermal Aging

255. **NEW METHODS FOR JOINING BETA”-ALUMINA TO NIOBIUM1%ZIRCONIUM FOR ALKALI METAL THERMAL TO ELECTRIC CONVERTERS (AMTEC)**
$100,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
AMPS Contact: T. Hunt (734) 677-4260

During this Phase I SBIR Program, number of approaches to sealing beta”-alumina to metal and insulator components for Alkali Metal Thermal to Electric Converter (AMTEC) cells were evaluated. The two most promising seal approaches were: 1) Use of a thin wall tapered metal sleeve seal, with the metal matched to the dimensions and thermal expansion coefficient of the two ceramics, alpha- and beta”-alumina; 2) the use of a tapered seal design incorporating a high temperature, sodium resistant, glass/ceramic filler material to join a beta”-alumina tube to a tapered alpha-alumina (or sapphire) collar, which, in turn, is pressed or wrung into a mating tapered metal socket in the tube support plate of the converter. Testing of tapered sleeve seals in power producing AMTEC cells showed performance equivalent to that of cells with hermetic, brazed seals.

Keywords: Ceramic-to-Metal Joining, AMTEC

256. **AMTEC ELECTRODE AND BETA”-ALUMINA SOLID ELECTROLYTE DEVELOPMENT**
$300,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
Texas A&M University Contact: M. Schuller (979) 845-8767

The development of improved performance electrode materials, principally iridium (rhenium) and mixed conductor electrode materials, was continued for potentially improved performance AMTEC cells.

Keywords: Electrode Materials, AMTEC

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

257. **FABRICATION DEVELOPMENT AND MATERIALS PRODUCTION FOR AMTEC CONVERTERS**
$800,000
DOE Contact: Dirk Cairns-Gallimore (301) 903-3332
ORNL Contact: J. F. King (865) 574-4807

This Advanced Radioisotope Power System (ARPS) Program has been developing the alkali metal thermal to electric (AMTEC) converter for power conversion in generators for outer planetary space missions of NASA.

ORNL has contributed to this Program in the areas of refractory metal alloy production, welding and brazing fabrication development and production of converters, measurement of total hemispherical emittance and thermal conductivity, magnetron sputtering of electrode coatings on BASE tubes, and studies of oxidation kinetics.

In FY2001, Vacuum-arc melted Mo-41%Re was produced to supply the stock material required for fabrication and development of AMTEC converters. Two ingots of the alloy were extruded, rolled to various thicknesses, and heat treated. Welding procedures were developed and several converters were fabricated. Brazing development was initiated to identify an alloy for joining alumina insulators to Mo-41%Re for converter feed throughs. Two Base tubes were sputtered with W-Rh for evaluation of the coating process.

Keywords: Molybdenum, Rhenium, Welding and Brazing, AMTEC

OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION

NUCLEAR ENERGY PLANT OPTIMIZATION

Nuclear Energy Plant Optimization projects are designed to address issues associated with aging management and plant performance optimization of light water reactors. The projects address both non-destructive testing, and the mechanical properties of structural components and cabling.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

258. **STEAM GENERATOR NDE TEST MOCKUP FACILITY**
$350,000
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contact: J. Benson (650) 855-2146
ANL Contact: D. Kupperman (630) 252-5108

To provide suitable test specimens and databases of NDE and characterization results that can be used to develop improved NDE techniques and signal analysis methods for the detection and characterization of SCC in steam generator tubing and provide the capability to assess and demonstrate the effectiveness of such methods.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator

259. **ADVANCED EDDY-CURRENT INSPECTION SYSTEM FOR DETECTION AND CHARACTERIZATION OF DEFECTS IN STEAM GENERATOR TUBES**
$300,000
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contact: J. Benson (650) 855 2146
ANL Contact: T. Wei (630) 252-4688

Develop an advanced eddy-current inspection technique and data analysis methodology for more reliable detection and accurate sizing of defects in steam generator tubes, including repaired tubes.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator

260. **DEVELOP EMPIRICAL DATA TO CHARACTERIZE AGING DEGRADATION OF POLYMERS USED IN ELECTRICAL CABLE**
$327,000
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Develop empirical data to characterize the aging behavior of polymer materials in electrical cable insulation and jackets for the following environments; typical power plant conditions, R&D laboratory experimental conditions, and environmental qualification tests.

Keywords: Polymers, Aging, Irradiation, Electrical Insulation

261. **DEVELOP CONDITION MONITORING (CM) TECHNIQUES FOR ELECTRICAL CABLE**
$591,019
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Develop nondestructive or essentially-nondestructive, science-based, CM techniques for electrical cable insulation and jacket materials that are capable of characterizing the current condition of either a local section or an entire cable run using parameters (e.g., density) correlated to aging models or other well-defined criteria. Confirmation of ability of identification of damaged insulation via electrical testing in an ionizable gas environment and extension ionized gas testing to locate and characterize damage sites will also be included. Development of a distributed temperature and radiation monitoring system based on fiber optic transmission characteristics will also be evaluated.

Keywords: Aging, Irradiation, Electrical Insulation, Fiber Optics

262. **MECHANICAL BEHAVIOR OF IRRADIATED STRUCTURAL STAINLESS STEELS**
$407,000
DOE Contact: G. W. Morris (301) 903-9527

EPRI Contact: H. T. Tang (650) 855-2012
ANL Contact: D. L. Porter (208) 533-7659

Determine the mechanical behavior of irradiated structural stainless steels under conditions of interest to LWRs and to develop constitutive models describing the behavior that can be used to develop tools to predict component life, assess the results of NDE examinations and guide the timing of corrective actions.

Keywords: Austenitic Stainless Steel, Irradiation, Mechanical Properties, Modeling, Stress Corrosion Cracking

263. **FATIGUE MANAGEMENT**
$560, 638
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contacts: J. Carey (650) 855-2105, S. Rosinski (704) 547-6123 and B. Carter (704) 547-6019

Provide cost effective methods of evaluating the cyclic life of nuclear components, including the effects of reactor coolant environment, based on the safety margins of the ASME Code, and to provide utilities with appropriate "tools" to manage fatigue effects.

Keywords: Fatigue, ASME Code, Environmental Fatigue

264. **ASSESSMENT OF AGING EFFECTS ON COMPONENTS AND STRUCTURES FROM NUCLEAR POWER PLANTS**
$50,000
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contacts: J. Carey (650) 855-2105 and S. Rosinski (704) 547-6123
ORNL Contact: T. M. Rosseel (865) 574-5380
PNNL Contact: S. K. Sundaram (509) 373-6665

Obtain materials and components that have been in service in operating reactors to be used for comparison with laboratory aged materials to validate models for aging effects and nondestructive examination methods. Provide information on the significance of aging effects and the effectiveness of plant programs for managing aging effects.

Keywords: Aging, Non-Destructive Examinations, Modeling

265. **IRRADIATION-INDUCED SWELLING AND STRESS RELAXATION OF PWR REACTOR CORE INTERNAL COMPONENTS**
$630,713
DOE Contact: G. W. Morris (301) 903-9527
EPRI Contact: H. T. Tang (650) 855-2012

Characterize irradiation-induced void swelling and stress relaxation related degradation that could occur in operating reactors, and calibrate and extend the breeder reactor based swelling model for PWR applications.

Keywords: Irradiation-Induced Swelling, Stress Relaxation

NUCLEAR ENERGY RESEARCH INITIATIVE

Nuclear Energy Research Initiative projects are designed to address materials issues associated with advanced nuclear reactors. The projects address the development and characterization of fuel, structural materials, and waste forms.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

266. **NOVEL CONCEPTS FOR DAMAGE-RESISTANT ALLOY IN NEXT GENERATION NUCLEAR POWER SYSTEMS**
$560,000
DOE Contact: C. Thompson (301) 903-3918
PNNL Contact: S. M. Bruemmer (509) 376-0636

The objective of the research is to develop the scientific basis for a new class of radiation-resistant materials to meet the needs for higher performance and extended life in next generation power reactors. New structural materials are being designed to delay or eliminate the detrimental radiation-induced changes that occur in austenitic alloys, i.e., a significant increase in strength and loss in ductility (<10 displacements per atom (dpa)), environment-induced cracking (<10 dpa), swelling (<50 dpa), and embrittlement (<100 dpa). Non-traditional approaches are employed to ameliorate the root causes of materials degradation in current light water reactor (LWR) systems. Changes in materials design are based on mechanistic understanding of radiation damage processes and environmental degradation and the extensive experience of the principal investigators with core component response.

Keywords: Alloy Development, Ion Irradiation, Nuclear Reactor Materials

267. **ADVANCED CERAMIC COMPOSITES FOR HIGH-TEMPERATURE FISSION REACTORS**
$260,000
DOE Contact: C. Thompson (301) 903-3918
PNNL Contact: R. H. Jones (509) 376-4276

This research seeks to develop the understanding needed to produce radiation-resistant SiC/SiC composites for advanced fission reactor applications. Structural and thermal performance of SiC/SiC composites in a neutron radiation field depends primarily on the radiation-induced defects and internal stresses resulting from this displacement damage. The researchers are working to develop comprehensive models of the thermal conductivity, fiber/matrix interface stress and mechanical properties of SiC/SiC composites as a function of neutron fluence, temperature, and composite microstructure. This model will be used to identify optimized composite structures that result in the maximum thermal conductivity and mechanical properties in a fission neutron field.

Keywords: SiC, Ceramic Composites, Nuclear Reactor Materials, Mechanical Properties

268. **DEVELOPMENT OF IMPROVED BURNABLE POISONS FOR COMMERCIAL NUCLEAR POWER REACTORS**
$415,000
DOE Contact: C. Thompson (301) 903-3918
ORNL Contact: M. L. Grossbeck (865) 574-5065

Burnable poisons are used in nuclear reactors to aid in reactivity control and to reduce power peaking. The materials used at the present time suffer from two common disadvantages. The first is that the elements currently used, such as gadolinium and boron result in a small residual negative reactivity. Ideally, the burnable poison should be entirely depleted by the time the fuel is depleted. In fact, some burnable poison or isotopes that result from neutron absorption in the burnable poison remain at the time of fuel depletion and serve to limit the amount of fuel that can be used. The second is that boron transmutes to helium, which creates undesirable internal fuel pin pressures. Elimination or reduction of these two effects will lead to higher fuel burnup and longer core life resulting in lower cost of operation.

For many absorbing elements, such as gadolinium, it is isotopes other than the primary absorber that lead to residual reactivity. A goal of this research is to investigate the possibility of separating isotopes to isolate the absorbing isotope of interest, thus reducing or eliminating the residual reactivity. Absorbing elements such as samarium, gadolinium, dysprosium, and other identified candidates are being considered. State of the art two-dimensional computer codes will be used to determine the effects of the new burnable poisons, in both homogeneous and self-shielded configurations, on reactivity and core safety parameters. The second phase of the project will investigate isotope separation by the plasma separation process, and test separations will be attempted. In the final phase of the project, product forms determined from phase one will be fabricated using techniques of ceramic processing.

Keywords: Burnable Poisons, Nuclear Reactor Fuel

269. **FUEL FOR A ONCE-THROUGH CYCLE (TH, U) O_2 IN A METAL MATRIX**
$360,035
DOE Contact: C. Thompson (301) 903-3918
ANL Contact: S. M. McDeavitt (630) 252-4308

Metal-matrix cermet nuclear fuels have potential for use in a once through, high-burnup, proliferation resistant fuel cycle. This project combines the advantages to be gained from cermet fuel with the resources extension potential of the thorium oxide fuel cycle and the inherent proliferation resistance of mixed oxide ceramics. These advantages fit well with the DOE's focus on the development of Generation IV nuclear power systems and proliferation resistant fuel cycles. The goal of this project is to demonstrate the feasibility of a metal-matrix fuel comprising (Th,U) O_2 microspheres in a zirconium matrix that can achieve high-burnup and be directly disposed as nuclear waste.

Keywords: Nuclear Reactor Fuel, Cermet, Thorium Oxide

270. **ADVANCED PROLIFERATION RESISTANT, LOWER COST, URANIUM-THORIUM DIOXIDE FUELS FOR LIGHT WATER REACTORS**
$1,132,742
DOE Contact: C. Thompson (301) 903-3918
INEEL Contact: P. E. MacDonald (208) 525-9634

The overall object of this project is to evaluate the efficacy of high burnup mixed thorium-uranium dioxide (ThO_2-UO_2) fuels for light water reactors (LWRs). A mixed thoria-urania fuel that can be operated to a relatively high burnup level in current and future LWRs may have the potential to:

- improve fuel cycle economics (allow higher sustainable plant capacity factors),
- improve fuel performance,
- increase proliferation resistance, and
- be a more stable and insoluble waste product than UO_2.

One of the important goals of this project is to study fuels that would be assembly-for-assembly compatible with the fuel in current LWRs. This implies that both utilities and vendors would find this fuel acceptable for manufacturing and use in current LWRs, if the economics prove to be desirable.

Keywords: Thorium-Uranium Dioxide, Nuclear Fuel

271. **DEVELOPMENT OF A STABILIZED LIGHT WATER REACTOR (LWR) FUEL MATRIX FOR EXTENDED BURNUP**
$360,348
DOE Contact: C. Thompson (301) 903-3918
PNNL Contact: B. D. Hanson (509) 376-3760

The main objective of this project is to develop an advanced fuel matrix based on the currently licensed UO_2 structure capable of achieving extended burnup while improving safety margins and reliability for present operations. Burnup is currently limited by the fission gas release and associated increase in fuel rod internal pressure, fuel swelling, and by cladding degradation. Once fuels exceed a threshold burnup, a "rim" or high burnup structure (HBS) forms. The HBS is characterized by the development of a subgrain microstructure having high porosity and low thermal conductivity. It is believed that the lower thermal conductivity results in larger temperature gradients and contributes to subsequent fission gas release. Fuel designs that decrease the centerline temperature while limiting the HBS restructuring, thereby decreasing the fission gas release should be able to achieve higher burnup and even allow higher operating power for increased efficiency.

Research at Pacific Northwest National Laboratory (PNNL) has demonstrated that the soluble fission products and actinides present in the matrix of irradiated (spent) fuels stabilized the fuel matrix with respect to oxidation to U_3O_8. The higher the soluble dopant concentration, the more resistant the fuel has been to undergoing the restructuring of the matrix from the cubic phase of UO_2 to the orthorhombic U_3O_8 phase. In this project, the attempt is to utilize the changes in fuel chemistry that result form doping the fuel to design a fuel that minimized HBS formation. The use of dopants that can act as getters of free oxygen and fission products to minimize fuel-side corrosion of the cladding is also being studied.

In addition to the use of dopants, project researchers are studying techniques such as the use of large grain sizes and radial variations in enrichment to minimize HBS formation and fission gas release. In this project, a combination of modeling and experimental studies is being used to determine the optimum design.

Keywords: Uranium Oxide, Nuclear Fuel, Phase Stability

272. **AN INNOVATIVE CERAMIC CORROSION PROTECTION SYSTEM FOR ZIRCALOY CLADING**
$228,874
DOE Contact: C. Thompson (301) 903-3918
University of Florida Contact: R. H. Baney (352) 392-5167

The operational lifetime of current Light Water Reactor (LWR) fuel is limited by thermal, chemical, and mechanical constraints associated with the fuel rods being used to generate nuclear heat. A primary limiting factor of this fuel is the waterside corrosion of the zirconium based alloy cladding surrounding the uranium pellet. This research project intends to develop thin ceramic films with adhesive properties to the metal cladding in order to eliminate the oxidation and hydriding of Zircaloy cladding. The corrosion protection system will allow fuel to operate safely at significantly higher burnups resulting in major benefits to plant safety and plant economics.

A major technical challenge for coating a metal with a ceramic protection system is to develop a cohesive bond between the two materials. The differences between the thermal expansion of the ceramic coating and the thermal expanding metal can, if not properly addressed, interfere with the ceramic's ability to maintain a bond and thus maintain a protective layer.

Keywords: Zircaloy, Ceramic Coating, Corrosion, Nuclear Fuel

273. **A SINGLE MATERIAL APPROACH TO REDUCING NUCLEAR WASTE VOLUME**
$210,000
DOE Contact: C. Thompson (301) 903-3918
ANL Contact: J. V. Beitz (630) 252-7393

This project is developing an innovative single material, minimum volume approach for the selective sorption of metal ion radionuclides from aqueous waste solutions and creation of a final nuclear waste form that is suitable for long term storage or geological burial. The project is based on a chemically functionalized porous silica that is termed Diphosil. Diphosil was created as an ion exchange medium that selectively and nearly irreversibly sorbs highly charged metal ions, such as actinides, from appreciably acidic aqueous solutions. The chelating power of Diphosil is due to diphosphonic acid groups that are anchored to its silica surface via organic spacer groups. Approximately 90 percent of the weight of dry Diphosil is silica (SiO_2).

Underlying this project is the hypothesis that heating metal ion-loaded Diphosil in air will oxidize its organic content to water vapor and carbon dioxide and its phosphonic acid groups to phosphoric acid that would react with the sorbed metal ions to give metal phosphates. Based on literature reports of the properties of porous silica, it was further hypothesized that additional heating would either volatilize any excess phosphoric acid or cause it to react with the silica to form silicon phosphates. At still higher temperature, pore collapse should occur thereby microencapsulating and chemically fixing the sorbed metal ions in phosphate-rich metal phases in vitreous silica. Vitreous silica is one of the most radiation resistant glasses known.

Keywords: Nuclear Waste, Silica, Ion Exchange

274. **DEVELOPING IMPROVED REACTOR STRUCTURAL MATERIALS USING PROTON IRRADIATION A RAPID ANALYSIS TOOL**
$375,000
DOE Contact: C. Thompson (301) 903-3918
ANL Contact: T. R. Allen (208) 533-7760

The purpose of this program is to design advanced reactor materials with improved resistance to void swelling and irradiation assisted stress corrosion cracking (IASCC) using three principal methods: bulk composition engineering, grain boundary composition engineering, and grain boundary structural engineering. The focus of the first year was bulk compositional engineering in which five different alloying additions were made to a base Fe-18Cr-8Ni-1.25Mn alloy whose bulk composition corresponds to 304 stainless steel. This alloy was chosen as the reference alloy for the program because 304 stainless steel is known to be susceptible to both swelling and IASCC. In addition to the studies on bulk composition engineering, work commenced on the grain boundary structural engineering. Thermomechanical treatments were developed for the Fe-18Cr-8Ni-1.25Mn alloy that increased the fraction of coincidence site lattice (CSL) boundaries.

Each of the bulk composition alloying additions was chosen for a specific purpose. Fe-18Cr-40Ni-1.25Mn was chosen because higher bulk nickel concentration is known to reduce swelling, but its affect on IASCC is unknown. Fe-18Cr-8Ni-1.25Mn+Zr was chosen because Zr is an oversized element that might trap point defects and prevent swelling and grain boundary segregation. Fe-16Cr-13Ni-1.25Mn, Fe-16Cr-13Ni-1.25Mn+Mo, and Fe-16Cr-13Ni-1.25Mn+Mo+P were chosen to determine why 316 stainless steel is more resistant to swelling and IASCC than 304 stainless steel.

Keywords: Proton Irradiation, Swelling, Environmental Cracking, Alloy Development

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

275. **APPLICATION OF INNOVATIVE EXPERIMENTAL AND NUMERICAL TECHNIQUES FOR THE ASSESSMENT OF REACTOR PRESSURE VESSEL STRUCTURAL INTEGRITY**
$70,000
DOE Contact: C. Thompson (301) 903-3918
SNL Contact: T. Y. Chu (505) 845-3217

The lower head of the reactor pressure vessel (RPV) can be subjected to significant thermal and pressure loads in the event of a core meltdown accident. The mechanical behavior of the reactor vessel lower head is of importance both in severe accident assessment and the assessment of accident mitigation strategies. For severe accident assessment the failure of the lower head defines the initial conditions for all ex-vessel events, and in accident mitigation the knowledge of mechanical behavior of the reactor vessel defines the possible operational envelope for accident mitigation. The need for validated models of the lower head in accident scenarios is accomplished by well-controlled, well-characterized large-scale experiments simulating realistic thermal/mechanical loads to the reactor pressure vessel.

This project consists of both experimental and analytical efforts in investigating the structural integrity of reactor pressure vessels. Experiments simulating the thermal/mechanical loads to a reactor pressure vessel generate data that can be implemented into a finite element code, such as the commercially available code ABAQUS, to assess the ability of the code to capture the response of the pressure vessel to severe accident conditions. In addition, the pressure vessel material (SA533B1 steel) used in these experiments is prototypic of reactor PWR vessel material and is well characterized by material property testing as part of this program.

The NERI/NRC/OECD sponsored program consists of eight international partners: Belgium, Czech Republic, Finland, France, Germany, Spain and Sweden and the U.S. U.S. support is provided by the NRC and the Department of Energy NERI program. This experimental/ analytical program builds on the accomplishments of a previous NRC sponsored Lower Head Failure (LHF) program (NUREG/CR-5582). The current program is referred to as the OECD Lower Head Failure (OLHF) program to distinguish it from the previous program and to recognize the international participation of the OECD.

Keywords: Ferritic Steel, Mechanical Behavior, Reactor Pressure Vessel

276. **INNOVATIVE CHEMITHERMAL TECHNIQUES FOR VERIFYING HYDROCARBON INTEGRITY IN NUCLEAR SAFETY MATERIALS**
$354,067
DOE Contact: C. Thompson (301) 903-3918
Pacific-Sierra Research Corporation Contact:

L. R. Mason (703) 807-5668

This research and development program is designed to explore new methods of assessing current condition and predicting remaining life of critical hydrocarbon materials in nuclear power plant environments. Of these materials, “1E” safety cable insulation is the primary focus. Additionally, o-ring, seal, and lubricant products designed for nuclear applications round out the materials studied. This 3-phase applied research program is providing industry with new innovative methods and reference data to conduct pragmatic material condition-monitoring programs for a wide range of polymer-based products. Key research objectives (products) include a material-condition-monitoring database, optimization and standardization of various testing procedures, implementation of proven engineering development methodologies, and inter-technology correlation analyses. Milestones are defined by a 5-task work-breakdown schedule. Task 1 encompasses front-end R&D program activities and planning of additional tasks. Task 2 concerns identification of subject cable materials, their acquisition, accelerated aging, testing by a suite of chemithermal methods, and results reporting.

Keywords: Polymers, Aging

277. **CONTINUOUS-WAVE RADAR TO DETECT DEFECTS WITHIN HEAT EXCHANGER & STEAM GENERATOR TUBES**
$372,000
DOE Contact: C. Thompson (301) 903-3918
SNL Contact: Thurlow W. H. Caffey
(505) 844-4217

The overall objective of this three-year program is to design, fabricate, and demonstrate a complete defect-detection system using an in-tube radar (ITR) within a variety of steam-generator tubing typically found in nuclear-electric power plants. The ITR is fundamentally different from the eddy-current methods now in use because it is based on backscatter from a defect rather than the disturbance of current flow in the tube wall. An electric field, parallel to the axis of the tube, is transmitted into the tube wall, reflected from a defect, and returned to an internal receiver all operating in the near field. The fundamental premise is that the change in axial electric field caused by the defect will be distinguishable from the null field present in the absence of defects.

This first year’s work had the following research objectives:

Defect Modeling - Three-dimensional (3D) electromagnetic codes in cylindrical coordinates, including the transmitter, were needed to determine the backscatter from defects of different geometries, orientations, and wall locations.

Alignment Sensitivity - Preliminary modeling showed that there would be no transmission from the transmitter to the receiver if both were located exactly on the centerline of the tube. However, further modeling was needed to show that slight departures from the ideal coaxial geometry, consistent with mechanical tolerances, would still allow acceptable performance.

Prototype Design - Mechanical packaging, centering provisions, fiber-optic links, on-board power, antennas, amplifiers, and translation system designs had to begin both to provide some parameters needed for the above modeling codes, and to ensure timely completion of the project.

Keywords: Non-Destructive Testing, Cracking

278. **FUNDAMENTAL MECHANISMS OF CORROSION OF ADVANCED ZIRCONIUM BASED ALLOYS AT HIGH BURN-UP**
$690,777
DOE Contact: C. Thompson (301) 903-3918
Westinghouse Electric Company Contact:
R. G. Lott (412) 256-1061

The corrosion behavior of nuclear fuel cladding is a key factor limiting the performance of nuclear fuel elements. Improved cladding alloys, which resist corrosion and radiation damage, will facilitate higher burnup core designs. The objective of this project is to understand the mechanisms by which alloy composition, heat treatment and microstructure affect corrosion rate. This knowledge will be used to predict the behavior of existing alloys outside the current experience base (for example, at high burnup) and predict the effects of changes in operating conditions on zirconium alloy behavior.

Zirconium alloys corrode by the formation of a highly adherent protective oxide layer. The working hypothesis of this project is that alloy composition, microstructure and heat treatment affect corrosion rates through their effect on the protective oxide structure and ion transport properties. Therefore, particular emphasis has been placed on detailed characterizations of the oxides formed on a series of experimental alloys. The goal of this project is to identify these differences and understand how they affect corrosion behavior. To do this, several microstructural examination techniques including transmission electron microscopy (TEM), electrochemical impedance spectroscopy (EIS) and a selection of fluorescence and diffraction techniques using synchrotron radiation at the Advanced Photon Source (APS) are being employed.

Detailed characterizations of oxides are only useful if the observations can be linked to the corrosion behavior of the alloy. That link requires a model of the corrosion mechanism. The modeling effort is designed to organize the data from the characterization studies in a self-consistent manner and link those observations to the corrosion behavior. The ultimate objective of this project is to link the characterization and theoretical modeling efforts to yield improved alloy specifications.

Keywords: Zirconium, Corrosion, Synchrotron Radiation, TEM, Electrochemical Impedance Spectroscopy

279. **MONITORING THE DURABILITY PERFORMANCE OF CONCRETE IN NUCLEAR WASTE CONTAINMENT**
$156,894
DOE Contact: C. Thompson (301) 903-3918
Massachusetts Institute of Technology Contact: F. Ulm (617) 253-3544

Concrete is commonly employed in radioactive waste disposal as an effective construction material for containment barriers, liners, and encasement of containers. The objective of this research is to develop the scientific knowledge and the appropriate engineering tools required to evaluate and quantify the durability performance of nuclear waste concrete containment subjected to the pessimistic chemical degradation scenario of calcium leaching. Monitoring the durability performance means here the quantitative assessment, in time and space, of the integrity of the containment during the entire storage period and requires the consideration of the multiple couplings between diffusion-dissolution of calcium and deformation and cracking.

With regard to the time-scale, the durability design of waste containers needs to consider some reference scenario of chemical degradation, in particular the pessimistic one of calcium leaching by pure water. This design scenario refers to the risk of water intrusion in the storage system. For the reference scenario at hand, it is generally assumed that concrete is subject to leaching by permanently renewed deionized water acting as a solvent. The calcium ion concentration in the interstitial pore solution leads to dissolution of the calcium bound in the skeleton of Portlandite Crystals, $Ca(OH)_2$, and calcium-silica-hydrates (C-S-H), with sharp dissolution fronts. This calcium leaching leads to a degradation of the mechanical properties of concrete (material strength, Young's modulus). Cracks increase the diffusivity of the calcium ions through the structure, and can lead to an acceleration of the chemical degradation, and hence to an acceleration of the overall structural aging kinetics. This process can lead to a closed loop of accelerated structural degradation.

Keywords: Nuclear Waste, Concrete, Mechanical Properties, Leaching

280. **DETERMINISTIC PREDICTION OF CORROSION DAMAGE IN HIGH LEVEL NUCLEAR WASTE**
$226,156
DOE Contact: C. Thompson (301) 903-3918
SRI International Contact: G. Engelhardt (650) 859-3671

This research involves developing deterministic models and associated computer codes for predicting the evolution of corrosion damage to high level nuclear waste (HLNW) containers. Safe disposal of our nation's HLNW represents one of the greatest technical challenges of the twentieth and twenty-first centuries. The principal challenge is to ensure isolation of the waste from the biosphere for periods up to 10,000 years under conditions that can only now be estimated. The lack of existing databases for the corrosion of candidate alloys over times that represent even a small fraction of the intended service life means that we cannot rely on empirical methods to provide the design, materials selection, and reliability assessment information that is required to assure the public that the technology chosen for the disposal of HLNW is effective and safe. Instead, only strategies based on the employment of deterministic models can be used, because the natural laws (laws of conservation) that are the foundation of these models constrain the solutions to physical reality and are invariant with time.

Existing deterministic models of general and localized corrosion allow us to predict the accumulation of corrosion damage in many systems. However, these models must be customized for predicting damage in HLNW canisters in a tuff repository. Thus, the influence of radiolysis on the corrosion potential and hence on the corrosion rate, for example, must be included in the models. Particular attention must be given to repassivation phenomena, because they eventually determine the extent of damage. Attempts to quantitatively describe localized corrosion damage without proper consideration of repassivation phenomena greatly underestimate the service lives of containers. It is also important to customize the models to the conditions to which the containers are expected to be exposed over the their design lives.

The principal objectives of this project are to:

- Develop deterministic models and associated computer codes for predicting the evolution of corrosion damage (i.e., "integrate' damage) to HLNW containers in the Yucca Mountain repository. Corrosion processes that will be considered include general corrosion (oxidation), pitting corrosion, crevice corrosion, and stress corrosion cracking.

- Develop deterministic methods for extrapolating corrosion rate data obtained under "accelerate" laboratory conditions to the field.

- Use the models to predict the fates of containers after exposure in the repository under various conditions (e.g., humid air, Contact with dripping water, repository inundation).

It is evident that the first objective is the basis of the project, and that other objectives can be achieved only if deterministic models for predicting corrosion damage to HLNW containers are developed.

Keywords: Nuclear Waste, Corrosion

281. **EFFECTS OF WATER RADIOLYSIS IN WATER COOLED NUCLEAR REACTORS**
$284,072
DOE Contact: C. Thompson (301) 903-3918
University of Notre Dame Contact: S. M. Pimblott (219) 631-7151

The goal of this research program is to develop a model that describes the chemical effects of radiation on aqueous systems and on aqueous/solid interfaces at temperatures associated with nuclear power plants and the Advanced Light Water Reactor (ALWR). The program has four thrusts:

Radiation Chemistry Modeling - An experiment-and-calculation based model will be developed to predict yields of the oxidizing and reducing radicals and the molecular species H_2 and H_2O_2 in aqueous systems like those associated with the ALWR chemistry.

High Temperature and High LET Effects - Experiments will measure the effect of dose on yields of O_2 and H_2O_2 produced in radiolysis with g-rays electrons and with H^+, He^{2+} and O^{8+} (C^{6+}) ions.

Interfacial Effects of Radiation - Experiments will gather information about radiation effects at aqueous/oxide interfaces of importance in fields such as reactor pipe corrosion and in storage of spent nuclear fuel.

Low Energy Electrons at Zirconia and Iron Oxide Surfaces and Interfaces - UHV experiments performed at Pacific Northwest National Laboratory with low energy electrons and photons will be used to simulate the damage caused at interfaces caused by the cascade of reactive secondary electrons produced by high-energy radiation.

Keywords: Corrosion, Zirconia, Radiolysis, Radiation

282. **MAPPING FLOW LOCALIZATION PROCESSES IN DEFORMATION OF IRRADIATED REACTOR STRUCTURAL ALLOYS**
$382,000
DOE Contact: C. Thompson (301) 903-3918
ORNL Contact: K. Farrell (865) 574-5059

The materials from which nuclear power reactors are constructed, namely ferritic steels for pressure vessels, austenitic stainless steel for core internals and piping, and zirconium alloys for fuel cladding and tubing, are normally quite ductile and workable. They are ductile because they undergo plastic flow, or deformation, by the generation and movement of dislocations on slip planes within the atomic lattice of the metal. Many intersecting slip planes are operative. The dislocations can move from one slip plane to another and they become entangled into a three-dimensional network of dislocation cells. This ability to develop a network of dislocation cells ensures that the material work hardens and deforms in a homogenous manner. That ability is lost when the materials are exposed to the action of penetrating neutrons in the reactor. The neutrons create disturbed regions in the regular arrangement of atoms in the atomic lattice. These disturbed regions, or radiation damage clusters, impede the slip dislocations and inhibit the formation of dislocation cells. Instead, the deformation becomes localized in narrow bands or channels, and sometimes in twin bands. This intensification of strain and stress by dislocation channel deformation (DCD) changes the mechanical properties of the material and causes embrittlement. The degree of embrittlement is related to the nature and the details of the dominant deformation mode, which are functions of the radiation exposure and of the mechanical test conditions.

Most mechanical property data for use in design data banks is derived from tensile tests. Radiation damage raises the tensile yield strength and UTS, induces yield point drops in materials that do not normally show sharp yield points, reduces the work hardening rate and the elongation, and causes premature plastic instability and failure. All of these changes are now known or suspected to involve DCD but only a few quantitative correlations have been made. If such correlations are made in detail they can allow preparation of deformation mode maps in which the regions and boundaries of the deformation modes are plotted in terms of plastic strain and neutron fluence. Mechanical properties representing the different deformation modes can be overlaid on the maps, and the maps become pictorial repositories of knowledge relevant to the irradiation behavior of the materials. These maps will not only simplify, condense, verify and specify essential properties and applications limits for crucial reactor components, but they will add immeasurably to our understanding of the interplay between radiation damage microstructures, deformation modes and mechanical properties responses. They should bring cohesion and assurance into the processes of selection, assessment, and application of reactor materials. Presently, deformation mode maps for irradiated materials exist only for nickel and gold. The goal of this project is to determine deformation mode maps for A533B ferritic steel, 316 stainless steel, and Zircaloy-4 alloy.

Keywords: Mechanical Properties, Stainless Steel, Zircaloy, Radiation

283. **A NOVEL APPROACH TO MATERIALS DEVELOPMENT FOR ADVANCED REACTOR SYSTEMS**
$147,704
DOE Contact: C. Thompson (301) 903-3918
University of Michigan Contact: G. S. Was (734) 763-4675

Component degradation by irradiation is a primary concern in current reactor systems as well as advanced designs and concepts where the demand for higher efficiency and performance will be considerably greater. In advanced reactor systems, core components will be expected to operate under increasingly hostile (temperature, pressure, radiation flux, dose, etc.) conditions. The current strategy for assessing radiation effects for the development of new materials is impractical in that the costs and time required to conduct reactor irradiations are becoming increasingly prohibitive, and the facilities for conducting these irradiations are becoming increasingly scarce. The next generation reactor designs will require more extreme conditions (temperature, flux, fluence), yet the capability for conducting irradiations for materials development and assessment in the next 20 years is significantly weaker than over the past 20 years. Short of building new test reactors, what is needed now are advanced tools and capabilities for studying radiation damage in materials that can keep pace with design development requirements.

The most successful of these irradiation tools has been high-energy (several MeV) proton irradiation. Proton irradiation to several tens of displacements per atom (dpa) can be conducted in a short amount of time (weeks), with relatively inexpensive accelerators, and result in negligible residual radioactivity. All of these factors combine to provide a radiation damage assessment tool that reduces the time and cost to develop and assess reactor materials by factors of 10 to 100. What remains to be accomplished is the application of this tool to specific materials problems and the extension of the technique to a wider range of problems in preparation for advanced reactor materials development and assessment.

The objective of this project is to identify the material changes due to irradiation that affect stress corrosion cracking (IASCC) of stainless steels, embrittlement of pressure vessel steels and corrosion and mechanical properties of Zircaloy fuel cladding. Until such changes are identified, no further progress can be made on identifying the mechanisms and solving the problems. An understanding of the mechanisms will allow for the development of mitigation strategies for existing core components and also the development of radiation-resistant alloys or microstructures that are essential for the success of advanced reactor designs.

Keywords: Stress Corrosion Cracking, Proton Irradiation, Zircaloy, TEM

284. **AN INVESTIGATION OF THE MECHANISM OF IGA/SCC OF ALLOY 600 IN CORROSION ACCELERATING HEATED CREVICE ENVIRONMENTS**
$289,650
DOE Contact: C. Thompson (301) 903-3918
Rockwell Science Center, LLC Contact: J. Lumsden, III (805) 373-4136

The concentrated solutions and deposits in tube/tube support plate crevices of nuclear steam generators have been correlated with several forms of corrosion on the outer secondary side of Alloy 600 steam generator tubes including intergranular attack/stress corrosion cracking (IGA/SCC), pitting, and wastage. Crevice chemistries in an operating steam generator cannot be measured directly because of their inaccessibility. In practice, computer codes, which are based upon hypothesized chemical reactions and thermal hydraulic mechanisms, are used to predict crevice chemistry. The objective of the Rockwell program is to provide an experimental base to benchmark crevice chemistry models, to benchmark crevice chemistry control measures designed to mitigate IGA/SCC, and to model IGA/SCC crack propagation processes. The important variables will be identified, including the relationship between bulk water chemistry and corrosion accelerating chemistries in a crevice. One important result will be the identification of water chemistry control measures needed to mitigate secondary side IGA/SCC in steam generator tubes. A second result will be a system, operating as a side-arm boiler, which can be used to monitor nuclear steam generator crevice chemistries and crevice chemistry conditions causing IGA/SCC.

Keywords: Stress Corrosion Cracking, Nickel-Base Alloys, Corrosion, Steam Generator

285. **RANDOM GRAIN BOUNDARY NETWORK CONNECTIVITY AS A PREDICTIVE TOOL FOR INTERGRANULAR STRESS-CORROSION CRACKING**
$382,324
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: W. E. King (925) 423-6947

Intergranular stress corrosion cracking (IGSCC) is one of the most pervasive degradation modes in current light water reactor systems and is likely to be a limiting factor in advanced systems as well. In structural materials, IGSCC arising from the combined action of a tensile stress, a “susceptible” material, and an “aggressive” environment has been recognized for many years and the mechanisms widely investigated. Recent work has demonstrated that by sequential thermomechanical processing, properties, such as corrosion, IGSCC, and creep of materials can be dramatically improved. The improvements have been correlated with the fraction of so-called “special” grain boundaries in the microstructure. A mutli-institutional team comprising of researchers from Lawrence Livermore National Laboratory (LLNL), University of Michigan (UM), and General Electric Corporate Research & Development (GECRD) propose an alternative explanation for these observations: that the effect of grain boundary engineering is to break the connectivity of the random grain boundary network through the introduction of low energy, degradation resistant twins and twin variants. This collaborative science and technology research project is aimed at verifying the mechanism by which sequential thermomechanical processing ameliorates IGSCC of alloys relevant to nuclear reactor applications and prescribing processing parameters that can be used in the manufacture of IGSCC resistant structures.

Methods will be developed to quantify the inter-connectivity of the random grain boundary network, measure the interconnectivity of a series of materials where the interconnectivity has been systematically altered. Property measurements will then be performed on the materials and their performance rankings compared with the boundary network measurements, and e the materials characterized to correlate actual crack paths with the measurements of the random grain boundary network. These data, will be used to evaluate and improve the methods that have been chosen to describe the random grain boundary network. The characterization method will be tested by evaluating the interconnectivity of the random grain boundary network in a series of as-received materials, rank their expected performance, and compare the results with property measurements.

The major accomplishments of this project are expected to be 1) the determination that the random boundary network connectivity (RBNC) is a major driver of IGSCC in low to medium stacking fault energy austenitic alloys 2) the development of a predictive tool for ranking. IGSCC performance of these alloys and 3) the establishment of thermomechanical processing parameters to be applied in the manufacture of IGSCC resistant materials. The outcome of the project will be identification of a mitigation strategy for IGSCC in current LWR conditions that can then enable the development of economically and operationally competitive water-cooled advanced reactor systems.

Keywords: Microstructure, Grain Boundaries, Stress Corrosion Cracking, Thermomechanical Processing

286. **FUNDAMENTAL UNDERSTANDING OF CRACK GROWTH IN STRUCTURAL COMPONENTS OF GENERATION IV SUPERCRITICAL LIGHT WATER REACTORS**
$265,696
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: I. Balachov (650) 859-3238

This work will contribute to the design of safe and economical Generation-IV Supercritical Light Water Reactors (SCLWR) by providing a basis for selecting structural materials to ensure functionality of in-vessel components during the entire service life and estimating life-time of structural components under a variety of normal and offset operating conditions.
The objectives of the project are to:

- Increase understanding of the fundamentals of crack growth in structural components of Generation-IV SCLWR made of stainless steels and nickel base alloys at supercritical temperatures,
- Provide tools for assessing the influence of the operating conditions in power plants with supercritical coolant temperatures on the electrochemistry of different types of corrosion processes taking place in the coolant circuits of supercritical power plants,
- Measure material-specific parameters describing the material’s susceptibility to stress corrosion cracking and other forms of environmentally assisted degradation of structural materials at supercritical coolant conditions,
- Use these measurements to interpret the rate-limiting processes in the corrosion phenomena and as input data for lifetime analysis,
- Use the SRI-developed FRASTA (Fracture surface topography analysis) technique to obtain information on crack nucleation times and crack growth rates via analysis of conjugate fracture surfaces. Identify candidate remedial actions by which the susceptibility to stress corrosion cracking can be decreased.

A unique combination of two advanced techniques for studying material reliability will be used. Controlled Distance Electrochemistry (CDE) will allow us to determine in relatively short experiments a measurable material parameter that describes the transport of ions or ionic defects in the oxide films and that will be correlated with the susceptibility to cracking, using fracture surface topography analysis (FRASTA) to reconstruct the evolution of crack initiation and growth

Keywords: Crack Growth, Corrosion, Fracture Surface Topography Analysis, Controlled Distance

287. **ELECTROCHEMISTRY DEVELOPMENT AND VALIDATION OF TEMPERATURE DEPENDENT THERMAL NEUTRON SCATTERING LAWS FOR APPLICATIONS AND SAFETY IMPLICATIONS IN GENERATION IV NUCLEAR REACTOR DESIGNS**
$243,656
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: A I. Hawari (919) 515-4598

The University of Cincinnati (UC), Oak Ridge National Laboratory (ORNL), and the Institute Balseiro (IB) will perform theoretical, computational, and experimental investigations on temperature dependent neutron thermalization in moderating materials that are of major importance to the safety of nuclear systems. The objectives of this work are: to critically review the currently used thermal neutron scattering laws for various moderators and fuel cells as a function of temperature, to use the review as a guide in examining and updating the various computational approaches in establishing the scattering law, to understand the implications of the obtained results on the ability to accurately define the operating and safety characteristics (e.g., the moderator temperature coefficient) of a given reactor design—that is, to know not only the reactivity coefficients but also their errors, sensitivity coefficients and covariance matrices, to develop and generate new sets of temperature dependent thermal neutron scattering laws, S(a,b), either by an evolutionary process or by changing the models entirely (e.g., introducing the coherent part of the inelastic scattering or using the synthetic kernel approach), and finally to test and benchmark the developed models within the framework of a neutron slowing down experiment. In particular, the studies will concentrate on investigating the latest ENDF/B thermal neutron cross sections for reactor grade graphite, beryllium, beryllium oxide, zirconium hydride, high purity light water, and polyethylene at temperatures greater than or equal to room temperature. These materials are neutron moderators/reflectors that will be used in the development of Generation IV nuclear power reactors and in many applications in the nuclear science and engineering field. Of major importance is graphite, which is the moderator in the modular pebble bed reactor (MPBR) that is being examined internationally as a possible Generation IV power reactor, as the subcritical reactor in accelerator driven concepts, and as the incinerator of radioactive waste and weapon's plutonium. Furthermore, a newly developed highly conductive form of graphite, known as graphite foam, is currently under study as a reactor material. Added to that, these materials of interest in research reactors such as zirconium hydride (i.e., TRIGA), and in Nerva derivative power sources for space applications (e.g., zirconium hydride, Be and BeO reflectors).

Keywords: Neutron Thermalization, Moderating Materials, Generation IV Nuclear Power Reactors

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2001
NATIONAL NUCLEAR SECURITY ADMINISTRATION - GRAND TOTAL	$113,041,000
OFFICE OF NAVAL REACTORS	$74,200,000[1]
OFFICE OF DEFENSE PROGRAMS	$38,841,000
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	$38,841,000
SANDIA NATIONAL LABORATORIES	$19,238,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$9,491,000
Materials Development and Characterization	2,210,000
Materials Processing	2,190,000
Physics and Chemistry of Nanostructured Materials	1,500,000
Functional Materials for Microsystems: Smart Self-Assembled Photochromic Films	282,000
Self-Healing Molecular Assemblies for Control of Friction and Adhesion in MEMS	361,000
Self-Assembled Templates for Fabricating Novel Nano-Arrays and Controlling Materials Growth	312,000
Next-Generation Output-Based Process Control: An Integration of Modeling, Sensors, and Intelligent Data Analysis	257,000
Functional Materials for Electrochemomechanical Actuation of Micro-valves and Micro-Pumps	298,000
Switchable Hydrophobic-Hydrophilic Surfaces	352,000
All-Ceramic Thin-Film Battery	310,000
Biocompatible Self-Assembly of Nano-Materials for BIO-MEMS and Insect Reconnaissance	352,000
Nanoclusters for Supercapacitors	325,000
Assuring Ultra-Clean Environments in Micro-system Packages: Irreversible and Reversible Getters	342,000
Science Based Processing of Field-Structured Composites	300,000
In Situ Characterization of Soft Solution Processes for Nanoscale Growth	100,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,565,000
Enhanced Surveillance: Material Lifetimes	2,142,000
Dynamic Materials: High Pressure, Shock Physics, and Nanomechanics	500,000
Science of Materials Synthesis, Aging and Diagnostics	1,000,000
Effects of Microstructural Variables on the Shock Wave Response of PZT 95/5	321,000
Innovative Experimental and Computational Diagnostics for Monitoring Corrosion in Weapons Environments	212,000
Linking Atomistic Computations with Phase Field Modeling	192,000
A Combinatorial Microlab Investigation of Critical Copper-Corrosion Mechanisms	674,000
Wetting and Spreading Dynamics of Solder and Braze Alloys	474,000
Diagnostics for Joining Solidification/Microstructural Simulations	327,000
LIGA Microsystems Aging: Evaluation and Mitigation	360,000
Mechanics and Tribology of MEMS Materials	210,000

[1]This excludes $50.1 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION (continued)

	FY 2001
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
SANDIA NATIONAL LABORATORIES (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
Improved Materials Aging Diagnostics and Mechanisms Through 2D Hyperspectral Imaging Methods and Algorithms	272,000
Exploration of New Multivariate Spectral Calibration Algorithms	125,000
Making the Connection Between Microstructure and Mechanics	257,000
Physical Basis for Interfacial Traction - Separation Models	297,000
Mechanisms of Dislocation-Grain Boundary Interaction	264,000
First-Principles Determination of Dislocation Properties	151,000
Dynamics of Metal/ceramic Interfaces	160,000
Microstructural and Continuum Evolution Modeling of Sintering	227,000
Magnetic-Field Effects on Vacuum-Arc Plasmas	207,000
Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	143,000
Understanding Metal Vaporization from Transient High Fluence Laser Irradiation	50,000
INSTRUMENTATION AND FACILITIES	$1,182,000
Enhanced Surveillance: Advanced Analytical Techniques	900,000
Microscale Shock Wave Physics Using Photonic Driver Techniques	282,000
LOS ALAMOS NATIONAL LABORATORY	$15,330,000
Enhanced Surveillance Campaign	15,330,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$4,273,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,800,000
Engineered Nanostructure Laminates	1,400,000
Laser Damage: Modeling and Characterization	400,000
INSTRUMENTATION AND FACILITIES	$2,473,000
AFM Investigations of Biomineralization	113,000
Polyimide Coating Technology for ICF Targets	1,700,000
Beryllium Ablator Coatings for NIF Targets	300,000
Using Dip-Pen Nanolithography to Order Proteins and Colloids at Surfaces	360,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

The mission of the National Nuclear Security Administration is:

- To enhance United States national security through the military application of nuclear energy.
- To maintain and enhance the safety, reliability and performance of the U.S. nuclear weapons stockpile, including the ability to design, produce and test, in order to meet national security requirements.
- To provide the U.S. Navy with safe, militarily effective nuclear propulsion plants and to ensure the safe and reliable operation of those plants.
- To provide international nuclear safety and nonproliferation.
- To reduce global danger from weapons of mass destruction.
- To support U.S. leadership in science and technology.

OFFICE OF NAVAL REACTORS

The Deputy Administrator for Naval Reactors within the National Nuclear Security Administration is responsible for conducting requirements under Section 309(a) of the Department of Energy Organization Act which assigns civilian power reactor programs and all DOE naval nuclear propulsion functions. Executive Order 12344, as set forth in Public Law 106-65, stipulates responsibilities and authority of the Naval Nuclear Propulsion Program, of which the Deputy Administrator for Naval Reactors is a part.

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $124.3 million in FY2001. Approximately $50.1 million represents the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (202) 264-8124.

OFFICE OF DEFENSE PROGRAMS

The Deputy Administrator for Defense Programs within the National Nuclear Security Administration is responsible for carrying out national security objectives established by the President for nuclear weapons and assisting in reducing the global nuclear danger by planning for, maintaining and enhancing the safety, reliability and performance of the U.S. stockpile of nuclear weapons and associated materials, capabilities and technologies in a safe, environmentally sound, and cost-effective manner.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

288. **MATERIALS DEVELOPMENT AND CHARACTERIZATION**
$2,210,000
DOE Contact: Christian Mailhiot (202) 586-7831
SNL Contact: Duane Dimos (505) 844-6385

The Materials Development & Characterization effort addresses the need for materials with specific properties or performance characteristics to be used in the enduring stockpile. Projects emphasize achieving scientific understanding of how the materials properties depend on composition, microstructure, and preparation conditions. Research focuses on materials that can serve as direct replacements for those in current use whose availability is curtailed by sunset technologies or ES&H regulations, on new materials to simplify production or surveillance, on new technological solutions to current component functions, or on enhanced reliability or surety. Current areas of emphasis include new approaches for encapsulants, foams and adhesives, control of material structure from the nano- to the meso-scale to provide materials with new functionality, providing the scientific basis for optimizing the properties of ferroelectrics.

Keywords: Materials Properties, New Materials, Material Structure, Polymeric Materials, Ferroelectrics

289. **MATERIALS PROCESSING**
$2,190,000
DOE Contact: Christian Mailhiot (202) 586-7831
SNL Contact: Ken Wilson (925) 294-2497

The Materials Processing effort seeks to develop a fundamental understanding of new and existing processes that are anticipated to be critical for defense programs needs. The effort emphasizes developing the understanding that will enable us to fabricate parts faster, with fewer defects, and at lower cost. The results of this effort are used to develop advanced manufacturing techniques for component production. One current area of emphasis is in Joining/Solidification Science, which seeks to develop fundamental understanding required to enable the predictive capability needed for solidification processes in manufacturing including welding, active brazing, melting, and casting, used in the production of non-nuclear components. The other area of emphasis, which is Advanced/Innovative Processes, seeks to develop a fundamental understanding of the relationship between processing conditions, microstructure, and properties for cold spray, thermal spray, ceramic sintering, and LIGA microfabrication.

Keywords: Advanced Manufacturing Techniques, Joining, Solidification, Sintering, LIGA Microfabrication

290. **PHYSICS AND CHEMISTRY OF NANOSTRUCTURED MATERIALS**
$1,500,000
DOE Contact: Christian Mailhiot (202) 586-7831
SNL Contact: Wil Gauster (505) 284-3504

In order to assure the performance and longevity of surety solutions for stockpile refurbishments, the fundamental physical and chemical behaviors of nanostructured materials are being investigated for materials with direct or potential use in surety components. Areas of investigation include nanostructured materials for innovations in microsystem design including new structural materials and materials for enhanced energy storage; developing and understanding surface modification and thin film deposition to tailor surface hardness, wear, friction, adhesion, optical and electrical properties; scientifically tailored lubricants and molecular level tribology; scientific basis for adhesion and stiction in dormant microsystems; atomic level control of compound semiconductor material synthesis, growth of self-assembled nanostructures and novel semiconductor materials, device processing and fabrication for reliable, high performance optoelectronic, microelectronic,and photonic devices; exploration of novel nanoelectronic and nanophotonic device concepts based on quantum effects in lower dimensions; developing and determining the range of validity of first-principles computational methods to describe the defect properties and dynamic response of materials.

Keywords: Nanomaterials, Nanocomposites, Microsystems, Tribology, Coatings, Compound Semiconductors, Computational Modeling

291. **FUNCTIONAL MATERIALS FOR MICROSYSTEMS: SMART SELF-ASSEMBLED PHOTOCHROMIC FILMS**
$282,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Terry A. Michalske (505) 844-5829

The objective is to develop smart interfacial films and 3-D composite nanostructures to exhibit photochromic responses to specific, highly-localized chemical and/or mechanical stimuli, and to integrate them into optical microsystems. The project will involve the design of functionalized chromophoric self-assembled materials that possess intense and environmentally-sensitive optical properties (absorptance, fluorescence) enabling their use as detectors of specific stimuli and transducers when interfaced with optical probes. Particularly strong material candidates are the conjugated polydiacetylenes. The organic functional material will be immobilized in an ordered, mesostructured inorganic host matrix, which will serve as a perm-selective barrier to chemical and biological agents and provide structural support for improved material durability. Multi-task scanning probe techniques (atomic force microscopy, near-field scanning optical microscopy) offering simultaneous optical and interfacial force capabilities will drive the chromophoric materials with localized and specific interactions for detailed characterization of physical mechanisms and parameters. The composite films will be directly interfaced with microscales devices as optical elements (e.g., intracavity mirrors, diffraction gratings), taking advantage of the very high sensitivity of device performance to real-time dielectric changes in the films.

Keywords: Microsystems, Self-Assembly, Photochromic Materials

292. **SELF-HEALING MOLECULAR ASSEMBLIES FOR CONTROL OF FRICTION AND ADHESION IN MEMS**
$361,000
DOE Contact: Gerald Green (202) 586-8377
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Major barriers to implementing MEMS technologies are the ability to chemically passivate and lubricate the surface of micromechanical structures to prevent adhesion and reduce friction and wear, and to prevent electrostatic charging of devices in radiation environments. We will develop a new class of molecular coatings that offer Si surface passivation, elimination of surface oxide layers, self-healing lubrication properties, and a built-in mechanism to release shear energy through reversible chemical cleavage. Two approaches will be investigated, first separately, then in combination. We will investigate molecular assemblies that form liquid crystalline lamellar structures with robust mechanical properties, and a novel method of chemically modifying the polycrystalline Si surface directly, without an intermediary oxide layer, in a process that occurs simultaneously with the etching step used to remove the sacrificial oxide. Used separately, the first method may improve high shear stress micromachine performance, while the second may be suitable for applications where adhesion control is critical. Most exciting is combining both methods, where the self-healing lubricant is used to form a protective layer over the chemically treated surface prepared by the second method. Mechanical stress studies on these materials at the nanometer scale will be performed using both new and existing scanning probe techniques. We will also employ molecular dynamics simulation techniques to calculate the lubricants response to shear and compressive forces, determine the molecular mechanisms involved, and propose lubricant structures by understanding the molecular structure-function relationship.

Keywords: Microsystems, Friction and Adhesion Control

293. **SELF-ASSEMBLED TEMPLATES FOR FABRICATING NOVEL NANO-ARRAYS AND CONTROLLING MATERIALS GROWTH**
$312,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Robert Q. Hwang (925) 294-1570

Novel and exciting phenomena which have the potential to revolutionize science, materials, next-generation production methods are manifested as structural dimensions approach the nanometer level. However, advances in lithography are insufficient to achieve this feature scale. As a result, molecular self-assembly has attracted a great deal of interest, since this provides a possible spontaneous mechanism by which nanometer sized arrays can be formed without mechanical intervention. Although these low tech processes are highly dependent on system/material specifics, new techniques and the science which underlies them can be developed in a manner that allows extension of the natural order of self-assembling systems. The approach is based on previous work in which we fabricated templates of unprecedented size and regularity. These templates will then be applied to form nano-arrays based on a wide range of materials with tunable properties and nano-scale selective area over-growth patterns for improving the materials quality of thin films.

Keywords: Self-Assembly, Nano-Materials, Materials Growth

294. **NEXT-GENERATION OUTPUT-BASED PROCESS CONTROL: AN INTEGRATION OF MODELING, SENSORS, AND INTELLIGENT DATA ANALYSIS**
$257,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Mark F. Smith (505) 845-3256

The goal of process-based quality is to accept WR (weapon reserve) product without inspection. For simple processes, traditional feedback control of process input variables might achieve this goal. However, input-based (upstream) control systems are a major source of DP production problems for complex processes. With recent advances in sensor technology, process modeling, intelligent data analysis, and computing power, a broadly applicable next-generation control technology that monitors and controls process output rather than input may now be possible. For real-time, output based (downstream) process control, it is necessary to rapidly interpret and correctly respond to large amounts of temporally and spatially varying data, which requires an innovative new approach to data analysis. Highly complex relationships between process inputs and outputs must also be correctly modeled, and cost-effective robust sensors must be developed. In addition, relationships between sensor observations and product microstructure, properties and performance must be understood and integrated into the control system. For some complex processes, e.g., thermal spray, a first-generation downstream process controller based on in-flight monitoring and control of the spray plume may be achievable because some of the requisite technology already exists. To extract needed information from large, rapidly varying, complex data in real-time, we will create a statistical methodology that combines response surface modeling with multivariate statistical process control and a modified simplex search algorithm that incorporates the concept of dynamic annealing.

Keywords: Process Control, Sensors, Process Modeling, Intelligent Data Analysis

295. **FUNCTIONAL MATERIALS FOR ELECTROCHEMOMECHANICAL ACTUATION OF MICRO-VALVES AND MICRO-PUMPS**
$298,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: William Even (925) 294-3217

It is generally recognized that integrated microsystems for DP applications, chemical sensing, and medical devices will not be possible without development of fast and efficient microactuators that can be used as valves and pumps. Conventionally actuated devices can affect the operating characteristics of microsystems and cannot be miniaturized without significant loss in performance. We propose to take advantage of ElectroChemoMechanical (ECM) functions of conductive polymers to be used as the work-producing unit in microactuators. The focus of the work is threefold. First, molecular structure and composition of conductive polymer gels will be tailored to maximize physical/mechanical response to electrochemical stimulation. Secondly, computational modeling, a key component of this proposal, will complement the formulation development. Lastly, polymer actuator geometry and microelectrodes will be designed, build and tested to optimize microscale performance.

Keywords: Microsystems, Sensors, Microactuators, Conducting Polymers

296. **SWITCHABLE HYDROPHOBIC-HYDROPHILIC SURFACES**
$352,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Terry Michalske (505) 844-5829

The objective of this work is to investigate the use of tethered organic coatings as a means of reversibly switching the surface chemistry of components in microanalytical systems. The specific target of the project involves the development of thin films that can be switched between hydrophilic and hydrophobic states with potential application for controlled pumping of fluids on a chip. The project involves learning how to: 1) synthesize switchable polymers and attach them to surfaces 2) optimize methods for stimulating desired configuration changes within the tethered polymers 3) develop methods for probing whether desired configuration changes occur and how such changes impact surface chemistry 4) model desired transitions in polymer phases and surface chemistries to aid in polymer and interface optimization, and 5) develop model microfluidic structures that can be used to evaluate coating performance for microanalytical systems. Scientific benefits of the project involve: 1) obtaining a deeper of surface solvation and what makes surfaces exhibit properties such as hydrophobic or hydrophilic states, and 2) obtaining insights into how polymers interact with solvents such as water, impacting topics ranging from polymer swelling to protein folding. Technical benefits of the project involve learning how to integrate new "smart" materials and nanostructures into microanalytical systems.

Keywords: Microanalytical, Switchable Polymers, Microfluidic, Solvation, Organic Coatings

297. **ALL-CERAMIC THIN-FILM BATTERY**
$310,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: B.G. Potter (505) 844-9919

The production of a thin-film, all-ceramic battery for power sources that generate the necessary power and energy to operate microsystems without substantially increasing the size of the device are required to achieve autonomy. However, thin-film batteries are currently inadequate to operate the microsystems effectively. We are developing a rechargeable thin-film All-Ceramic Lithium-Ion Battery (ACB) using solution route deposition methods. The ACB will have higher power output, longer run times, and a greatly simplified production scheme in comparison to existing technology. Several ACB prototypes (normal and inverted) have been generated using the above chemistries; however, shorting has complicated the electronic testing. Once sufficiently developed, these ACB will have the versatility to power any number of small systems, such as microsystems and miniature autonomous robotics.

Keywords: Batteries, Microsystems, Thin Films, Lithium Ion Battery

298. **BIOCOMPATIBLE SELF-ASSEMBLY OF NANO-MATERIALS FOR BIO-MEMS AND INSECT RECONNAISSANCE**
$352,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: B.G. Potter (505) 844-9919

Living cells integrate, within a very small volume, recognition, amplification, and transduction properties of interest for environmental sensors. Key to practical cell-based sensors is patterned cell immobilization in robust, biocompatible, environments that maintain cell viability and accessibility while enabling signal transduction and transmittal. Bulk silica matrices formed by 'classical' sol-gel processing have been used for cell entrapment, but alcohol solvents cause protein denaturization, and, upon drying, broad pore size distributions lead to the collapse of small pores and the complete drying-out of large pores, limiting accessibility or causing cell inactivation. Furthermore, bulk gels are difficult to integrate into devices like MEMS. Evaporation-induced self-assembly (EISA) employs surfactants to direct the self-assembly of silica into periodic structures characterized by unimodal pore sizes and 1-, 2-, or 3-D connectivity of pore channel networks that are stable during drying. Using ink-jet printing, we can pattern these pore network systems on arbitrary surfaces. Unfortunately all surfactant structure-directing agents used to date are bio-incompatible at concentrations needed for self-assembly. This project explores new biocompatible self-assembly approaches to enable both incorporation of whole cells into microelectromechanical systems (MEMS) architectures and the writing of functional nanostructures on living reconnaissance agents. Through genetic modification, cell-based sensors can be developed for specific CW, BW or explosive threats.

Keywords: Nanostructure, Self Assembly, MEMS, Ink-Jet Printing, Sensors

299. **NANOCLUSTERS FOR SUPERCAPACITORS**
$325,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: George Samara (505) 844-6653

High current and voltage capacitors, such as those used in weapons systems, use polymer films as dielectric materials. The dielectric constant of these polymer films is very low, limiting the energy storage of these capacitors. Because the energy requirements are high for weapons components, these capacitors are large, occupying a significant fraction of device volume, and leaving little room for the diagnostic devices that are now envisioned. One route to freeing up space is to create a capacitor film dielectric with a much higher dielectric constant, which would result in smaller capacitors if the dielectric strength can be maintained. We are investigating whether high dielectric constant nanoparticles can be used to significantly increase the dielectric constant of a capacitor material and thus energy storage in film capacitors. This idea is motivated by our ability to make narrow dispersity nanoparticles of controlled sizes from 1.6-10 nm that are atomically smooth and have a precisely controlled organic capping layer thicknesses. These nanoparticles should be able to increase the dielectric constant of a capacitor film by a factor of five. If such a principle applies to both organic and inorganic dielectrics, a large commercial demand is anticipated, for products ranging from supercapacitors to improved automotive ignition components.

Keywords: Nanoparticles, Supercapacitors, Dielectric Constant, Polymer Films

300. **ASSURING ULTRA-CLEAN ENVIRONMENTS IN MICRO-SYSTEM PACKAGES: IRREVERSIBLE AND REVERSIBLE GETTERS**
$342,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: William Even (925) 294-3217

Microsystems are currently being evaluated as possible replacements for a number of weapon subsystems with the expectation of improved surety combined with reduced weight and volume. However, there is great concern that long periods of dormant storage may impair the mechanical functioning of microdevices that are exposed to water, out gassing products and particulates. Low-temperature operating environments and small moving parts in contact with stationary and mating structures make capillary condensation, ice formation and corrosion true concerns for microsystems. We are developing a new generation of irreversible, chemically reacting getters specifically targeted toward assuring the integrity of the local environment within microsystem packages. We intend to incorporate reactive volatile species into a polymer through covalent bonds, thus producing a non-volatile product. These reactive getters will be combined with getters that rely on absorption media (e.g. zeolites and high surface area carbon fibers) to scavenge non-reactive species, like solvents. Our getter systems will rely on device packaging to limit exchange between the microsystem and the global weapon environment. Thus, the internal getters need only provide local environmental control within the microsystem package. Modeling and analysis of available data will be used to estimate the ingress of undesirable species as well as the gettering rates, capacities, and geometries needed to maintain an acceptable environment within the package.

Keywords: Getter, Microdevices

301. **SCIENCE BASED PROCESSING OF FIELD-STRUCTURED COMPOSITES**
$300,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Richard Salzbrenner (505) 844-9408

Over the past few years, a new class of materials called Field-Structured Composites (FSCs) has emerged that poses interesting and novel process control challenges. FSCs are anisotropic particle composites produced in electric or magnetic fields, that exhibit highly anisotropic properties due to the chain or sheet-like structures that form as a result of the induced dipolar forces between particles. The field structuring gives tremendous control of material properties, and the potential for practical applications is great if feedback can be used to tailor material properties to meet specific needs. Recent research at Sandia has shown that these materials have colossal thermoresistance, piezoresistance, magnetoresistance, and chemiresistance, making FSCs very promising as sensors, if reliably produced with a desired resistivity. These materials pose nontrivial feedback control challenges, due to strong history effects, diverging time scales, and nonlinear dynamics. We propose to meet these challenges by developing science-based process control using newly discovered methods of achieving feedback in these materials. This involves using a rotating "destructuring" magnetic field to disrupt previously established structures that give rise to strong hysteresis in the sample conductivity-field strength response curve. The goal is to precisely control conductivity in samples during polymerization, or during solvent evaporation from samples where metal particles have been introduced into a polymer matrix through swelling. These systems pose exceptionally challenging control problems because the particle dynamics occur on diverging time scales.

Keywords: Field Structuring, Composites, Thermoresistance, Piezoresistance, Magnetoresistance, Chemiresistance

302. ***IN SITU* CHARACTERIZATION OF SOFT SOLUTION PROCESSES FOR NANOSCALE GROWTH**
$100,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Nelson Bell (505) 844-6234

The study of novel materials and structures with dimensions in the nanoscale (<100 nm) regime is an important, emerging field of materials science. The small size of these materials results in quantum confinement and surface contributions that translate into novel opto-electronic properties whose applications are still being realized. Many synthesis techniques for nanomaterials are based on soft solution processes (SSP), which include sol-gel, hydrothermal, solvothermal, micellular or organic templating routes, and electrochemical methods. These processes involve the precipitation of ionic species or metal-organic molecules into nanoparticles or nanostructured networks. In order to exercise a high degree of control over these processes, it is critical to have a capability for following the development of supersaturation, surface processes, and formation of a precipitating system *in situ*. This proposal will study the superposition of different measurement techniques to characterize dynamic colloidal systems in novel ways. These studies will probe the chemical interactions during reactions, and the organizational characteristics developed in the resulting colloids.

Keywords: Nanomaterials, Soft Solution Processes, Colloids

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

303. **ENHANCED SURVEILLANCE: MATERIAL LIFETIMES**
$2,142,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Richard J. Salzbrenner (505) 844-9408

The Material Lifetimes effort addresses the chemical and physical mechanisms that cause materials properties to change with time. The time-dependent properties of non-nuclear materials will be determined in the weapon storage environment and under other accelerated and natural aging conditions. The distribution in behavior caused by composition and processing variability and by variability in weapon storage/transport/use environments will be determined and their impact on weapon systems requirements for safety and performance will be established. The fundamental understanding of degradation processes in metals used in stockpile weapons will be advanced and this knowledge used to develop predictive models of failure due to corrosion, diffusion, microstructural evolution, and thermo-mechanical fatigue. Work on metals and metal interfaces will quantify interface performance requirements and develop validated predictive models for their behavior as a function of time and environment. A predictive understanding of the highest risk failure modes due to aging of organic materials will be developed.

Keywords: Materials Aging, Reliability, Corrosion, Metal Interfaces, Time-Dependent Properties

304. **DYNAMIC MATERIALS: HIGH PRESSURE, SHOCK PHYSICS, AND NANOMECHANICS**
$500,000
DOE Contact: Christian Mailhiot (202) 586-7831
SNL Contact: George Samara (505) 844-6653

An objective of this work is to develop continuum and atomic level understanding for models of shock-induced phenomena in materials necessary for shock-activated weapons components. Together with complementary high-pressure material physics studies, the research provides new understanding of ferroelectrics and polymeric encapsulants as well as essential insights to guide performance and reliability assessments, simulation capabilities and device improvements. A specific task is to develop sufficient understanding of the effects of induced porosity in the shock response of PZT 95/5 ceramic to guide optimization of pore former type and quantity during material production. We also develop and implement new experimental techniques for investigating performance and failure characteristics of power supply configurations at extreme temperatures. On a more fundamental level, we are working to improve our understanding of the relaxational responses of mixed perovskite ferroelectrics and encapsulates. An additional objective is to develop a precise understanding of the high strain-rate behavior of materials of interest for weapons systems, which requires materials processing and modeling at the atomic level. For modeling, code development and implementation is being done to understand the mechanical properties of materials, and ultimately to link electronic and atomic-level properties to the continuum level. For experimentation, new methodologies of producing atomically-tailored materials and testing the mechanical response of these materials are being explored.

Keywords: Ferroelectrics, Shock Physics, Power Supplies, Performance Modeling, Nanomaterials

305. **SCIENCE OF MATERIALS SYNTHESIS, AGING AND DIAGNOSTICS**
$1,000,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Wil Gauster (505) 284-3504

This effort is focused on identifying and studying the aging behavior of non-nuclear components in weapons systems, and developing relevant diagnostic techniques. It includes identifying the physics needed to model aging processes and developing models for the aging of components. Current emphasis is on experimental measurements and modeling of micromachine material surfaces and interfaces to provide the understanding needed to improve silicon MEMS and LIGA performance and aging characteristics. Properties of interest include stiction, friction, wear, and susceptibility to corrosion. To provide a basic understanding, we develop validated models for the chemical processes involved in synthesis and aging of thin films. An example of this work is the identification of physical and chemical effects of humidity on the structure of alkylsiloxane lubricant layers for silicon MEMS. We also provide predictive multi-scale (atomistic to continuum) models for corrosion and other processes involving chemically reacting heterogeneous materials, including corrosion of electrical components. We conduct hydrogen occluder film materials science research to insure the optimum performance and aging of existing and new designs of neutron tube (NT) sources and targets for the stockpile.

Keywords: Materials Aging, Reliability, Corrosion, Microsystems, Thin Films, Surface Science

306. **EFFECTS OF MICROSTRUCTURAL VARIABLES ON THE SHOCK WAVE RESPONSE OF PZT 95/5**
$321,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: George Samara (505) 844-6653

Sandia has responsibility for the design and production of neutron generators. Most generators use explosively driven power supplies in which shock wave depoling of the ferroelectric ceramic PZT 95/5 provides the required high voltage for the neutron tube. Generator production will change within a few years to PZT 95/5 material prepared using a new "chem prep" process that is still under development. This process will introduce a porous microstructure that is significantly different than that found within most material presently in the stockpile. Early studies showed that the porous microstructure can have a profound effect on performance: the rate for failures due to high-voltage breakdown at low temperatures is acceptably low only in materials made within a narrow density range through the addition of organic pore formers. More fundamentally, the dielectric and ferroelectric properties of the material and the physics of the FE (ferroelectric)-to-AFE (antiferroelectric) phase transformation that governs the depoling process depend on microstructural properties in ways that are not well understood. This project represents the first systematic study of the basic physics of microstructural effects on PZT 95/5 electromechanical behavior under shock loading. Dielectric properties are characterized for material samples having different densities, and the electromechanical responses of similar samples are investigated under carefully controlled shock loading conditions. Results to date demonstrate significant porosity effects on both the dynamic material response and shock-induced depoling, provide insight into a recently confirmed failure mechanism, and underscore the continuing need for systematically examining microstructural variables.

Keywords: Shock Wave Depoling, Ferroelectric, PZT 95/5, Phase Transition

307. **INNOVATIVE EXPERIMENTAL AND COMPUTATIONAL DIAGNOSTICS FOR MONITORING CORROSION IN WEAPONS ENVIRONMENTS**
$212,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Jeff Braithwaite (505) 844-7749

Reducing the size scale at which we measure and understand corrosion-based degradation pathways is of primary importance to scientific stewardship of the enduring stockpile. Central to this goal is to understand atmospheric degradation of Al based alloys. Galvanic interactions play a primary role in atmospheric degradation of 1) Al alloys due to electrochemically active second phase particles and 2) high purity Al used in microelectronics due to intimate contact with more noble metals (i.e., Au bond pads). A mechanistic understanding of the atmospheric electrochemical failure modes requires a precise spatial description of potential and current within a corroding system. Measuring the potential field and resulting current map on a small length scale in an adsorbed electrolyte is not possible using conventional electrodes and measurement techniques. We have taken a two-pronged approach to developing adequate electrodes. The first relies on our expertise in nano-engineering techniques and yields thin film electrodes. The second uses more traditional components such as thin metal foils and small diameter wires. We are constructing electrodes that allow for passive measurement of material interactions as well as providing the means for conducting true 3-electrode electrochemical experiments in adsorbed water layers. Results of these experiments provide inputs to a 3-D electrical field model, which can then predict the corrosion behavior of more complex systems.

Keywords: Corrosion, Electrodes, Potential Field

308. **LINKING ATOMISTIC COMPUTATIONS WITH PHASE FIELD MODELING**
$192,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Eliot Fang (505) 844-4526

The phase field model has proven to be a very powerful tool for modeling microstructural evolution during complex materials processing techniques. Although the method can be used to study grain growth and particle coarsening, the phase field model is particularly effective in predicting dendrite formation and solute redistribution during solidification and is therefore very useful in the numerical modeling of joining operations– welding, soldering and brazing. To date most of the work utilizing the phase field concept has focused on the development of the numerical technique and the study of generic microstructures; microstructure modeling applied to specific alloy systems has been rare. The lack of direct comparison between model predictions and actual microstructures in real alloys stems from the fact that many materials parameters-mobilities, free energies, surface energies, gradient energy coefficients, etc.—required as input in the phase field model and often these parameters are difficult to obtain experimentally. The purpose of this project is to employ atomistic calculations to obtain numerical values of all parameters necessary to model microstructural evolution. We will concentrate our efforts on the Cu-Ni system, which represents a model-brazing alloy.

Keywords: Computational Materials Science, Modeling of Materials Properties

309. **A COMBINATORIAL MICROLAB INVESTIGATION OF CRITICAL COPPER-CORROSION MECHANISMS**
$674,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Charles Barbour (505) 844-5517

An important aspect in developing a capability to predict stockpile reliability is a physics-based understanding of atmospheric corrosion. Corrosion modeling is hindered by limited knowledge of primary mechanisms and large numbers of coupled chemical reactions, which depend on complex interactions of materials with environment and functionality. This multidimensional problem requires fundamentally new experimental approaches, which can provide timely quantitative information on critical phenomena occurring in corrosion phase space. We are combining parallel miniature experimentation with ultrasensitive microanalytical techniques to efficiently explore this phase space and identify mechanisms and kinetics for copper sulfidation in the Microdomain Laboratory. This approach differs from convention by focusing on microscopic length scales, the relevant scale for corrosion. Combinatorial experiments (arrays of microlabs) will quantify the direct and synergistic effects of morphological and metallurgical variables (alloying, defect density in the Cu oxide and bulk, diffusivities, porosity), environmental variables (sulfur content in air, light exposure, water droplet size and distribution versus humidity), and functionality (e.g., electric-current conduction). Novel diagnostics include conductivity microsensors to locally quantify pH_2O and pH_2S, *in situ* electrical conductivity and light scattering to monitor real-time evolution of corrosion reactions, local ion-selective potentiometric monitoring of reaction products, and ultimately microcalorimetry sensors.

Keywords: Corrosion, Combinatorial Techniques

310. **WETTING AND SPREADING DYNAMICS OF SOLDER AND BRAZE ALLOYS**
$474,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Neal Shinn (505) 844-5457

The purpose of this project is twofold: 1) to develop a scientific understanding of the microscopic processes that control wetting and spreading dynamics in materials systems related to soldering and brazing; and 2) to design improved active braze alloys by investigating the thermodynamic aspects of reactive wetting of eutectic silver-copper alloys on ceramic substrates. The first task exploits new advances in experimental surface techniques and atomistic modeling methods to study wetting and spreading phenomena on length scales that range from Angstroms to microns. The unique imaging capabilities of the low energy electron microscope (LEEM) and scanning tunneling microscope are being used to characterize the interfacial region when materials such as Pb and Sn are deposited on Cu surfaces. We also use LEEM to observe the spreading behavior of small molten droplets on fully characterized metal surfaces. Results from these studies are used to test the validity of atomic potentials being developed to simulate the dynamics of wetting and flow. We currently have accurate, empirical potentials that can be applied in large-scale simulations involving Pb, Cu, and Ag. In the second task we develop new active-metal-braze alloy compositions based on thermodynamic considerations and test the proposed materials for improved performance. The goal is to achieve strong, hermetic seals in the brazing of kovar to alumina. Fundamental investigations of active braze materials on model alumina surfaces under well-controlled conditions and realistic simulations will provide a science-based approach for the design of improved, active-braze materials.

Keywords: Braze Alloys, Reactive Wetting, Low Energy Electron Microscope, Atomic Potential, Hermetic Seals

311. **DIAGNOSTICS FOR JOINING SOLIDIFICATION/MICROSTRUCTURAL SIMULATIONS**
$327,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Mark F. Smith (505) 845-3256

Solidification is an important aspect of welding, brazing, soldering, LENS fabrication, and casting. For these processes solidification affects, and in many instances controls, the final microstructure and properties of the product. The current trend toward utilizing large-scale process simulations and materials response models for simulation-based engineering is driving the development of new modeling techniques. However, the effective utilization of these models and simulations is currently limited by a lack of fundamental understanding of the sub-processes and interactions involved. This project is identifying key physical phenomena in, and expanding and refining our mechanistic descriptions of, solidification in the Fe-Cr-Ni system. The experimental study is coupled to modeling efforts focused on solidification processes in the same alloy system, and provides necessary mechanistic descriptions and input data for these models. We have developed and will continue to refine new and expanded experimental techniques, particularly those needed for *in situ* measurement of the kinetics features of the solidification process. This approach has identified several unexpected features of the solidification process, including the observation that the solidification front is more dynamic than previously thought and the observation of a previously unreported orientation relationship between ferrite and austenite.

Keywords: Solidification, Ferrite, Austenite, Joining

312. **LIGA MICROSYSTEMS AGING: EVALUATION AND MITIGATION**
$360,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Jill Hruby (925) 294-2596

The deployment of LIGA structures in DP applications requires a thorough understanding of potential long-term physical and chemical changes that may occur during service. While these components are generally fabricated from simple metallic systems such as copper, nickel and nickel alloys, the electroplating process used to form them creates microstructural features which differ from those found in conventional (e.g. ingot metallurgy) processing of such materials. Physical changes in non-equilibrium microstructures may occur due to long-term exposure to temperatures sufficient to permit atomic and vacancy mobility. Chemical changes, particularly at the surfaces of LIGA parts, may occur in the presence of gaseous chemical species and contact with other metallic structures. We propose to characterize LIGA materials, including pure Ni, Ni-Co and Ni-Fe alloys. This baseline characterization will be used as a reference point as we monitor changes that occur in LIGA structures over extended time periods in environments similar to those envisioned for DP applications. Finally, conformal coating systems will be investigated as needed to combat environmental degradation occurring at LIGA surfaces.

Keywords: LIGA, Electroplating, Non-Equilibrium Microstructures

313. **MECHANICS AND TRIBOLOGY OF MEMS MATERIALS**
$210,000
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Micromachines have the potential to significantly impact future weapon component designs as well as other defense, industrial, and consumer product applications. For both electroplated (LIGA) and surface micromachined (SMM) structural elements, the influence of processing on structure, and the resultant effects on material properties are not well understood. The behavior of dynamic interfaces in present as-fabricated microsystem materials is inadequate for most applications and the fundamental relationships between processing conditions and tribological behavior in these systems are not clearly defined. We intend to develop a basic understanding of deformation, fracture, and surface interactions responsible for friction and wear of microelectromechanical system (MEMS) materials. This will enable needed design flexibility for these devices, as well as strengthen our understanding of material behavior at the nanoscale. The goal of this project is to develop new capabilities for sub-microscale mechanical and tribological measurements, and to exercise these capabilities to discover fundamental knowledge of material behavior at this size scale. Novel micro-force and displacement sensors using SMM technology and new methodologies for isolating local variations in mechanical response of MEMS materials will be developed. Increased understanding of MEMS mechanics and tribology developed in this project will permit performance and reliability of advanced MEMS components to be predicted with a sound scientific basis.

Keywords: Micromachines, Interfaces, Tribology, Surface Interactions

314. **IMPROVED MATERIALS AGING DIAGNOSTICS AND MECHANISMS THROUGH 2D HYPER-SPECTRAL IMAGING METHODS AND ALGORITHMS**
$272,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Nancy Jackson (505) 845-7191

Twenty years ago, we developed new quantitative multivariate spectral analysis methods that caused a quantum leap in the capabilities of quantitative spectroscopy over previous univariate methods. We have now achieved a more significant revolution in the capabilities of quantitative spectral analyses. By combining the massive amounts of data generated using new commercial 2-dimensional (2D) infrared (IR) imaging spectrometers with the Sandia invention of powerful new hyperspectral information extraction algorithms, we have developed the ability to perform quantitative spectroscopy without the need for calibration standards. Thus, we can now rapidly obtain 2D spectral images of aging polymeric and energetic materials and directly extract pure-component spectra of all spectrally active chemical species in samples, which include the spectra of degradation products. This information combined with our new hyperspectral analysis algorithms can allow us to obtain accurate compositional maps of materials with ~10-micrometer spatial resolution. This new work has been able to directly impact materials degradation diagnostics by distinguishing multiple aging mechanisms and by greatly improving infrared sensitivity and chemical selectivity. The chemical specificity and spatial mapping of 2D IR spectroscopy will allow quantification of degradation products to help understand degradation mechanisms, kinetics, and diffusion.

Keywords: Multivariate Spectral Analysis, Hyperspectral Information Extraction, IR Spectroscopy, Chemometrics

315. **EXPLORATION OF NEW MULTIVARIATE SPECTRAL CALIBRATION ALGORITHMS**
$125,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Nancy Jackson (505) 845-7191

Previously we developed a powerful new multivariate calibration algorithm that has the ability to correct many of the outstanding limitations of traditional quantitative multivariate spectral calibrations such as minimizing the numbers of calibration samples and maintaining calibrations in the presence of drift. While investigating the limitations of this new algorithm, we developed a family of better algorithms that have the ability to be rapidly updated during prediction without recalibration. This rapid updating feature is a significant advantage over previous approaches and can impact weapon projects and industrial problems where spectral quality control and/or process monitoring is desired. The new algorithms have been demonstrated to improve the quantitative hyperspectral image analyses of aged materials. However we need to better understand the relative merits of these new multivariate algorithms and the relative performance of the new methods compared to traditional multivariate calibration methods. We also need to explore a variety of potential applications using the new algorithms. For example, the new algorithms may be able to 1) improve the qualitative information in the derived pure-component spectra of complex samples, 2) rapidly update multivariate spectral calibration models for changes in starting products for commercial process monitoring or quality control, and 3) improve hyperspectral image analyses from many sources including remote sensing.

Keywords: Multivariate Calibration, Hyperspectral Image

316. **MAKING THE CONNECTION BETWEEN MICROSTRUCTURE AND MECHANICS**
$257,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Eliot Fang (505) 844-4526

The purpose of microstructural control is to optimize materials properties. To that end, we have developed sophisticated and successful computational models of both microstructural evolution and mechanical response. However there is currently no way to couple these models to quantitatively predict the properties of a given microstructure. The problem arises because continuous response models, such as finite element, finite volume, or materials point methods, do not incorporate a real length scale. In this project, we are taking a tiered risk approach to incorporate microstructure and its resultant length scales in mechanical response simulations. The successful coupled model will predict both properties as a function of microstructure and microstructural development as a function of processing conditions.

Keywords: Microstructure, Mechanical Properties, Computational Materials Science

317. **PHYSICAL BASIS FOR INTERFACIAL TRACTION - SEPARATION MODELS**
$297,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: David Reedy (505) 844-3297

Many components contain interfaces between dissimilar materials where cracks can initiate and fail components. In recent years, researchers in the fracture community have adopted a cohesive zone model for simulating crack propagation (based upon traction-separation relations). Sandia is implementing this model in its ASCI codes. However, one important obstacle to using a cohesive zone modeling approach is that traction-separation relations are chosen in an ad hoc manner. The goal of the present work is to determine a physical basis for mesoscale level Traction-Separation (T-U) relations. We propose experiments that will elucidate the dependence of such relations on adhesive and bulk properties. Work will focus on epoxy/solid interfaces, although the approach is applicable to a broad range of materials. The crucial roles of crack tip plastic zone size and interfacial adhesion are being defined by varying epoxy layer thickness and using coupling agents or special self-assembled monolayers (SAMs) in preparing samples. The nature of the yield zone will be probed in collaborative experiments run at the Advanced Photon Source, and high-resolution optical methods will be used to measure crack opening displacements of the SDCB specimens. This work will provide an understanding of the major mesoscale phenomena governing polymer/solid interfacial fracture and identify the essential features that must be incorporated in a T-U based cohesive zone failure model. We believe that models using physically based T-U relations will provide an essential tool for using models to tailor interface properties to meet design needs.

Keywords: Traction-Separation, Interfacial Fracture

318. **MECHANISMS OF DISLOCATION-GRAIN BOUNDARY INTERACTION**
$264,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Robert Hwang (925) 294-1570

Incorporating the localized atomistic and microscopic effects of internal interfaces on materials properties and long-term behavior is a significant challenge for large-scale materials simulations. Critical to improving such models is developing an improved understanding of the dislocation-grain boundary interactions that ultimately control the interfacial response to strain. Such interactions impact many materials phenomena and properties including slip transmission, boundary migration, recrystallization, and yield strength and are a critical element in linking atomic structure to continuum behavior. In this project we seek to develop an experimentally based understanding of these dislocation-grain boundary interactions.

Keywords: Dislocation, Grain Boundary

319. **FIRST-PRINCIPLES DETERMINATION OF DISLOCATION PROPERTIES**
$151,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Robert Hwang (925) 294-1570

Dislocation behavior determines numerous materials properties. Their motion produces deformation. The interaction of dislocations with interfaces produces the grain-size dependence of strength. Motion of dislocations in boundaries determines the boundary mobility and thereby microstructural evolution. Prediction of dislocation core structures at the atomistic level in arbitrary materials and ultimately in the presence of defects is central to developing predictive models of material evolution. The need to treat arbitrary materials, alloys and dopants requires a predictive first-principles approach. Current first-principles modeling capabilities are not well suited to the description of dislocation properties. Techniques for determining the electronic structure of large numbers of atoms (order-N methods) work well for insulating materials but not for metallic systems. Further, essentially all *ab-initio* modeling to date employs band structure techniques with periodic boundary conditions. Thus dislocations and other aperiodic defects are difficult to model. We will adapt a combined electronic/lattice Green's technique to the direct calculation of dislocation core structures, which avoids the requirement of periodic boundary conditions. Both Green's functions exploit the short-range character of the Hamiltonians defining them. Additional modeling using an *ab-initio* extension of Peierls-Nabarro is also being pursued. The result of these calculations can be validated by detailed comparison with high-resolution electron microscopy observations. The success of this project will create a new world-class tool for the fundamental study of dislocation properties.

Keywords: Dislocations, First-Principles Modeling, Hamiltonians,

320. **DYNAMICS OF METAL/CERAMIC INTERFACES**
$160,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Robert Hwang (925) 294-1570

The goal of this project is to understand how metal/ceramic interfaces form, evolve, and accommodate the stress that can lead to delamination and failure. We emphasize the use of advanced microscopies such as scanning-tunneling microcopy and low-energy-electron microscopy to observe interface formation in real time. These techniques are used to measure the interfacial work of adhesion, determine the mechanisms and kinetics of interface formation, and develop understanding of how stress is or is not accommodated.

Keywords: Metal/Ceramic Interfaces, Microscopy, Adhesion

321. **MICROSTRUCTURAL AND CONTINUUM EVOLUTION MODELING OF SINTERING**
$227,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Eliot Fang (505) 844-4526

All ceramics and powder metals, including the ceramic components that Sandia uses in critical weapons components, are sintered, which is one of the most critical processing steps during ceramic manufacturing. Microstructural evolution, macroscopic shrinkage, and shape distortions during sintering will control the engineering performance of the resulting ceramic component. Yet, modeling and prediction of sintering behavior is in its infancy, lagging far behind the other manufacturing models. This project will develop a set of computational tools that will enable us to understand, predict, and control microstructural evolution and macroscopic dimensional changes during sintering. Previous research efforts on sintering modeling have failed because they treat some limited aspect of sintering, either on the microstructural or macroscopic continuum scale. We propose to develop a novel modeling method that can treat the microstructural evolution of thousands of powder particles during sintering and integrate the results into continuum models to predict the overall shrinkage and shape distortions in a sintering component. An equally important result of this work will be a fundamental advancement in the understanding of sintering science.

Keywords: Sintering, Ceramic Manufacturing, Microstructural Evolution, Manufacturing Models

322. **MAGNETIC-FIELD EFFECTS ON VACUUM-ARC PLASMAS**
$207,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Gerald Hays (505) 844-4135

Compact neutron tubes employ annular ion beams to minimize adverse effects due to the space charge of ions in the beam. Presently, annular beams are formed by geometrically selecting a fraction of the total output from vacuum-arc plasma ion sources. In principle, magnetic fields can be used to shape the plasma into an annular shape, thereby increasing source efficiency and reducing electrical drive requirements, which implies reduced generator size and weight. Moreover, self-magnetic fields of the arc affect the plasma output, but are not included in existing models of tubes. In the first year of project, we have begun development of diagnostics and codes to help us understand the field-plasma-arc interaction and to shape the plasma plume. We propose to continue employing a combination of modeling and experiment to understand and exploit our measurements and to design new field configurations to shape the plasma as desired. The modeling has begun, including 3-D computations of plasma response to magnetic fields with an existing plasma code [Large-Scale Plasma code (LSP)]. Experimental diagnostics under development include Langmuir-probe arrays configured to provide comprehensive 3-D plasma-mapping capability. We have started measurements with simple 1-D fields for code validation, and will extend the work to the complex 3-D fields of the arc and complex coil systems. This work will improve our understanding of important tube processes and will allow Sandia to tailor the spatial distribution of plasma for better utilization and increased margin in tubes.

Keywords: Vacuum-Arc Plasmas, Magnetic Fields, Plasma Plume, Langmuir Probe

323. **DETERMINATION OF CRITICAL LENGTH SCALES FOR CORROSION PROCESSES USING MICROELECTROANALYTICAL TECHNIQUES**
$143,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Jeff Braithwaite (505) 844-7749

A key factor in our ability to produce and predict the stability of metal-based macro- to nano-scale structures and devices is a fundamental understanding of the localized nature of corrosion. Corrosion processes where physical dimensions become critical in the degradation process include localized corrosion initiation in passivated metals, micro-galvanic interactions in metal alloys, and chemistry in adsorbed water films in atmospheric corrosion. This work focuses on two areas of corrosion science, where a fundamental understanding of processes occurring at critical dimensions is not currently available. We will study the critical length scales necessary for passive film breakdown in the inundated Al system and the chemical reactions and transport in ultra-thin water films relevant to the atmospheric corrosion of Al. We will combine low current measurements with microelectrodes to study the size scale required to observe a single initiation event and record electrochemical breakdown events. The resulting quantitative measure of stability will be correlated with metal grain size, secondary phase size and distribution to understand which metal properties control stability at the macro- and nano-scale. Mechanisms of atmospheric corrosion on Al are dependent on the physical dimensions and continuity of adsorbed water layers as well as the chemical reactions that take place in this layer. We will combine microelectrode arrays with electrochemical sensing and electrostatic force microscopy to monitor the chemistry and ion transport in these thin layers. The techniques developed and information derived from this work will be used to understand and predict degradation processes in electrical and structural components.

Keywords: Corrosion Science, Microelectrodes, Degradation Processes

324. **UNDERSTANDING METAL VAPORIZATION FROM TRANSIENT HIGH FLUENCE LASER IRRADIATION**
$50,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Mark F. Smith (505) 845-3256

Laser spot welding is widely used for precision joining of nuclear weapon components and is a strong candidate to be employed for joining micro-machines . However, the production of metal vapor as a consequence of high-fluence laser irradiation is a serious concern in cleanrooms. Despite the widespread use of lasers for the welding of high-value-added components, little fundamental understanding of laser/material interaction exists. Laser spot welding experiments are planned to quantify the effect of laser pulse parameters on weld pool dimensions and liquid metal expulsion propensity. In addition, we intend to refine previous laser weld characterization techniques and develop new approaches for quantifying the temperature field in laser spot welds, primarily through careful measurement of alloy element vaporization rates. Development of these analysis techniques provides a needed foundation for model prediction of laser weld pool vaporization.

Keywords: Laser Welding, Laser/Material Interaction

INSTRUMENTATION AND FACILITIES

325. **ENHANCED SURVEILLANCE: ADVANCED ANALYTICAL TECHNIQUES**
$900,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Richard J. Salzbrenner (505) 844-9408

The Advanced Analytical Techniques effort supports the development of advanced methods of characterizing materials structure and providing chemical analysis. The purpose of this work to develop the analytical techniques that will enable the detection and quantification of the chemical and physical mechanisms, that cause materials properties to change with time. Areas of emphasis include: 1) microstructural techniques using electron and X-ray beams to perform structural, chemical, and phase analysis on the nanometer to micron scale; 2) development of new information extraction algorithms to take advantage of hyperspectral data and other very large data sets; 3) optical and mass spectrometry techniques to probe subtle chemical changes that take place as materials in weapon systems age.

Keywords: Materials Structure, Chemical Analysis, Phase Analysis, Information Extraction Algorithms, Hyperspectral Data

326. **MICROSCALE SHOCK WAVE PHYSICS USING PHOTONIC DRIVER TECHNIQUES**
$282,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: George A. Samara (505) 844-6653

The goal of this project is to establish a new capability for conducting shock wave physics experiments at low per-experiment costs through a reduction in experimental length and time scales. Based on the earlier development of laser-driven optical detonators at Sandia, this new capability utilizes the rapid absorption of optical energy from a large, Q-switched, solid-state laser to accelerate a small, planar disk of a material of interest (a launch process known as photonic driving). The disk (or "flyer") subsequently impact another material, generating shock waves in both materials having amplitudes and durations that depend on the two materials, the impact velocity, and the disk thickness. Sub-nanosecond interferometric diagnostics were developed previously to examine the motion and impact of laser-driven flyers. To address a broad range of materials and stress states, photonic driving levels must be scaled up considerably from optical detonator conditions. However, progressively increasing concerns over laser-induced damage mechanisms in optics, thermally driven phase transitions and instabilities in laser-driven materials, and beam shaping requirements accompany the desire to scale up driving levels.

Keywords: Shock Wave Physics, Photonic Driver

LOS ALAMOS NATIONAL LABORATORY

327. **ENHANCED SURVEILLANCE CAMPAIGN**
$15,330,000
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LANL Contacts: J. Martz (505) 667-2323 and
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The Stockpile Surveillance Program provides protection to the U.S. nuclear weapons stockpile by an intensive program that assures it is free of defects that may affect performance, safety, or reliability. It consists of two elements, the Stockpile Evaluation Program and the Enhanced Surveillance Campaign. The Stockpile Evaluation Program provides the examinations and assessments of WR stockpile weapons and components. The Enhanced Surveillance Program provides means to strengthen the Stockpile Evaluation Program to meet the challenges of an aging stockpile in an era of no nuclear testing as well as providing lifetime assessments and predictions for SLEP planning.

The Enhanced Surveillance Campaign will protect the health of the stockpile by providing advance warning of manufacturing and aging defects to allow refurbishment before performance is impaired. The Campaign will provide diagnostics for screening of weapons systems to identify units that must be refurbished as well as for early detection of defects. It will also predict material and component aging rates as a basis for annual certification, refurbishment scope and timing, and nuclear weapon complex planning. Results of the work will include improvements to the basic Surveillance Program. Since nuclear weapons will be retained in the stockpile for lifetimes beyond our experience, the Department of Energy (DOE) needs a firm basis on which to determine when stockpile systems must be refurbished or reconditioned. If new refurbishment capability is needed, the DOE needs to know:

When these capabilities must be operational and what the required capacity should be;

- If the capacity for existing facilities is adequate and when potential refurbishment for the various stockpile systems must be scheduled;
- A basis from which to characterize the functional reliability of aged components, as part of the annual assessment process

The work in the ES Campaign began in late FY97 and will be completed at the end of FY08. The principal milestones and deliverables (Level 1) for this campaign are below:

- Provide component assessment annually for use in performing the annual assessment of the stockpile (FY02-08)
- Provide component lifetime assessments for weapon refurbishments to enable component replacement decisions and age-aware component design and material selections (FY03-06)
- Provide data or requirements to enable facility planning, design, and construction (FY02-06)
- Develop validated models for the aging of materials, components, and systems for use in weapon certification (FY03-07)
- Deliver advanced diagnostic tools to enable more predictive, higher fidelity, and non-destructive surveillance test capability (FY02-08)

Our work is divided into five major technical elements (MTE): pits, CSAs/Cases, high explosives (HE), systems, and non-nuclear materials (NNM). The pit, CSA/Cases, and high explosives MTEs are each divided into two projects; lifetime assessments and diagnostics. The Systems MTE is responsible for assessments/ methodologies to support decision making under uncertainty. The Non-nuclear materials MTE is divided into two projects; material lifetimes and advanced diagnostic tools.

Complete details for the Enhanced Surveillance Campaign can be found in the ESC Program plan and the ESC Implementation plan updated on a yearly basis.

Keywords: Nuclear Weapons, Pits, Plutonium, CSA, Canned Subassembly, High Explosives, Non-nuclear Materials, Systems, Reliability, Energetic Materials, Stockpile, Enhanced Surveillance, Campaign 8, Accelerated Aging, Lifetime Prediction, Aging

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

328. **ENGINEERED NANOSTRUCTURE LAMINATES**
$1,400,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contact: Troy W. Barbee, Jr.
(925) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one or two dimensions during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2nm) to hundreds of monolayers (>100nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500 mm thick samples have been synthesized for mechanical property studies of multilayer structures and energetic materials development.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately >50 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: EUV, soft X-ray and X-ray optics for spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; high strength materials; integrated circuit interconnects; machine tool coatings; projection X-ray lithography optics.

Keywords: Precision Thin Films; Multilayer Technology, Passive Elecrtonic Devices, IR, Visible, UV, EUV, SXR and XR Optics, Optic Systems

329. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contact: T. Diaz de la Rubia
(925) 422-6714

The objective of this project is to understand the mechanisms for laser-induced damage in optical materials used in high-peak-power laser systems such as the National Ignition Facility (NIF). The material system of primary interest is polished fused silica surfaces. The primary characterization tools used in the studies include luminescence spectroscopy and microscopy, total internal reflection microscopy (TIRM), near-field scanning optical microscopy (NSOM), and photothermal microscopy (PTM). Efforts are focused on the understanding of damage growth due to successive pulses and the mitigation of the growth through removal of the damaged material. The damage growth rate determines the functional lifetime of the optic in the laser system. The dependence of the damage growth rate on laser wavelength, pulse length, and pulse repetition rate is being determined. Also of interest is the influence of optic environment (air vs. vacuum) on the damage processes. Large-scale molecular dynamics simulations have been performed to study the behavior of fused silica glass under shocks induced by the laser beam. These simulations show a transformation in the structure of fused silica. An increase in density of about 20% is extracted from these calculations in agreement with experiments. They also show atomic level changes in the structure, in particular, changes in the ring-size distribution. This modified material could potentially have different optical properties. First principle calculations of the shocked material indeed show an increase in the absorption at the wavelength of interest. This increase in absorption could have consequences for damage growth during subsequent laser pulses. The results of these simulations are being compared with the experiments described above, in order to obtain a predictive model for damage production and growth in fused silica during laser irradiation.

Keywords: Silica, Luminescence, Laser Damage

INSTRUMENTATION AND FACILITIES

330. **AFM INVESTIGATIONS OF BIOMINERALIZATION**
$113,000
DOE Contact: Nick Woodward (301) 903-4061
LLNL Contact: J. J. DeYoreo (925) 423-4240

Living organisms use organic modifiers of nucleation and growth to control the location, size and shape of mineralized structures. While much is known about the macroscopic impact of these growth modifiers or has been inferred about the microscopic interfacial relationships between the modifiers and crystal surfaces, the atomic-scale mechanisms of biomineralization are poorly understood. In this project we use atomic force microscopy, molecular modeling and surface spectroscopy to investigate the effects of small inorganic and organic growth modifiers as well as proteins and their sub-segments on the growth of single crystal surfaces from solution. From these measurements we seek to determine growth mechanisms, geometrical relationships, and the effect on the thermodynamic and kinetic parameters controlling growth morphology and rate.

Keywords: Biomineralization, Atomic Force Microscopy, Crystal Growth

331. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$1,700,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. Cook (925) 422-3117 and Steve Letts (925) 422-0937

This program has as its objective the development of a vapor deposition based polyimide coating technology to produce a smooth 150 µm polyimide ablator coating on a 2mm diameter capsule target for the National Ignition Facility (NIF). The approach involves first vapor depositing monomeric species to form a polyamic acid coating on a spherical hollow mandrel. The surfaces of these coated mandrels are then smoothed by exposure to dimethyl sulfoxide vapor while being levitated on a nitrogen gas flow. The smoothed shells are then heated *in situ* to imidize the coatings. The focus of the past year has been improvement of the capsule surface finish.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

332. **BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS**
$300,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. McEachern (925) 423-4734, R. Cook (925) 422-3117 and R. Wallace (925) 423-7864

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 200 µm of a uniform, smooth, high-Z doped Be-based ablator on a spherical hollow mandrel. Capsules made with this type of ablator have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF). Emphasis in the past year has been on improving coating homogeneity and smoothness by reducing grain size and developing laser drilling techniques that will be needed for capsule filling.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

333. **USING DIP-PEN NANOLITHOGRAPHY TO ORDER PROTEINS AND COLLOIDS AT SURFACES**
$360,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contact: J. J. DeYoreo (925) 423-4240

The ability to organize nanometer scale species such as quantum dots, proteins, colloids and viruses is emerging as a key area of nanoscience and technology. In this project we are using dip-pen nanolithography to pattern surfaces at the nanoscale in order to create templates for assembly of ordered arrays. We are utilizing “inks” that covalently bind to the “paper” (i.e., the substrate) and that ensure chemo-selective binding of the target species to the pattern. By shrinking the pattern to sufficiently small size we will be able to assemble single molecules or colloidal species into well defined arrays. The degree of ordering in those arrays will then be investigated using synchrotron methods and the assembly process itself will be modeled using kinetic Monte Carlo simulations

Keywords: Dip-Pen Nanolithography, Atomic Force Microscopy, Templates, Nanoscale Patterns

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 2001
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT - GRAND TOTAL	$30,370,100
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$30,370,100
Waste Packages	$30,370,100

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

334. **WASTE PACKAGES**
$30,370,100
DOE Contact: Paige Russell (702) 794-1315
M&O Contacts: Larry Trautner, (702) 295-4414
and Robert Andrews (702) 295-5549

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Charactization Project Office. Bechtel SAIC Company, the contractor for the Civilian Radioactive Waste Management System, is responsible for designing the waste package and related portions of the engineered barrier system. The advanced conceptual design was completed in 1996 and Viability Assessment design was completed in 1998. The current design was selected in 1999. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF),canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE-owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. The current design consists of a corrosion-resistant outer barrier of alloy 22 and a stainless steel inner shell, which provides structural support. Titanium is still used as the drip shield material.

The waste package materials effort includes the testing and modeling of materials being considered for inclusion in the waste package and the engineered barrier system. These materials include Alloy 22 (UNS# N06022), titanium grade 7, and 316L stainless steel. The testing includes general aqueous and humid air testing, localized attack such as pitting and service corrosion, micro-biologically-influenced corrosion, galvanic corrosion, and stress corrosion cracking. The corrosion test facility started the long-term (at least five-year) test program in FY 1997. Evaluations of two year UNS# N06022 specimens were initiated and documented in project reports. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. In 1999 the short-term test program was continued to support waste package material degradation model development effort. The short-term test program focuses on stress corrosion cracking, hydrogen embrittlement, crevice corrosion, galvanic effects among the candidate materials and determination of the appropriate test environment that will represent saturated aqueous condition on the waste package surface.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF FOSSIL ENERGY

	FY 2001
OFFICE OF FOSSIL ENERGY - GRAND TOTAL	$10,568,000
OFFICE OF ADVANCED RESEARCH	$10,568,000
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM	$6,447,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,354,000
Fabrication Technologies for Fuel Cell Applications	110,000
Intermetallic Reinforced Cr Alloys	110,000
Corrosion Protection of Ultrahigh Temperature Metallic Alloys	200,000
Mo-Si Alloy Development	200,000
Development of Modified Austenitic Alloys	200,000
CRADAs on Advanced Alloy Development	18,000
CRADA on Thermie Alloy Processing	34,000
CRADA with INCO on High Creep Strength Alloys	50,000
Influence of Processing on Microstructure and Properties of Aluminides	170,000
Extended-lifetime Metallic Coatings for High-temperature Environmental Protection	210,000
Aluminide Coatings for Power-Generation Applications	85,000
Chemically-Vapor-Deposited YSZ for Thermal and Environmental Barrier Coatings	225,000
Corrosion-Resistant Composite Structures	275,000
Modeling for CVD of Solid Oxide Electrolyte	90,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils	76,000
Development of Hot Pressing as a Low-Cost Processing Technique for Fuel Cell Fabrication	4,000
Development of Novel Activated Carbon Composites	190,000
CRADAs for Development and Testing of Carbon Fiber Composite Molecular Sieves	107,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,511,000
Oxide Dispersion Strengthened (ODS) Alloys	390,000
Investigation of the Weldability of Intermetallics	70,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	20,000
Investigation of Iron Aluminide Weld Overlays	53,000
In-plant Corrosion Probe Tests of Advanced Austenitic Alloys	87,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	175,000
Reduction of Defect Content in ODS Alloys	78,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	60,000
Reliable Ceramic Coatings for High-Temperature Environmental Resistance in Fossil Environments	70,000
Development of Nondestructive Evaluation Methods for Structural Ceramics	175,000
Impermeable Thin Al_2O_3 Overlay for TBC Protection for Sulfate and Vanadate Attack In High Temperature Gas Turbines	333,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,582,000
Materials and Components in Fossil Energy Applications Newsletter	60,000
Development of Ceramic Membranes for Hydrogen Separation	350,000
Proton Exchange Membranes for Hydrogen Separation	2,000
Solid State Electrolyte Systems for Fuel Cells and Gas Separation	630,000
Improved Fuel Cell Materials and Economical Fabrication	184,000

OFFICE OF FOSSIL ENERGY (continued)

	FY 2001
OFFICE OF ADVANCED RESEARCH (continued)	
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
Bismuth Oxide Solid Electrolyte Oxygen Separation Membranes	125,000
Metallic Filters for Hot-Gas Cleaning	90,000
Refractory Materials Issues in Gasifiers	100,000
Pd-Ag Membranes for Hydrogen Separation	100,000
High-Temperature Materials Testing in Coal Combustion Environments	200,000
Molecular Sieves for Hydrogen Separation	150,000
Oxide-Dispersion-Strengthened Fe_3Al-Based Alloy Tubes	50,000
Development of ODS Alloy for Heat Exchanger Tubing	106,000
Fatigue and Fracture Behavior of Cr-X Alloys	30,000
Management of the Fossil Energy Advanced Research Materials Program	400,000
Personal Services Contract	5,000
ADVANCED METALLURGICAL PROCESSES PROGRAM	$3,822,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$862,000
Advanced Foil Lamination Technology	562,000
Continuous Casting of Titanium	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,960,000
Advanced Refractories for Gasifiers	600,000
Oxidation and Sulfidation Resistant Materials	1,160,000
Erosion and Wear	600,000
Mechanisms of Corrosion Under Ash Deposits	400,000
Non-Isothermal Corrosion and Oxidation	200,000
ULTRA-SUPERCRITICAL POWER PLANT RESEARCH	$299,000
Materials for Ultra-Supercritical Steam Power Plants	299,000

OFFICE OF FOSSIL ENERGY

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil, and natural gas) research and development program. This research is generally directed by the Office of Coal Technology, the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

1. The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.

2. The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.

3. The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM

Fossil Energy materials-related research is conducted under the Advanced Research Materials Program. The goal of the Fossil Energy Advanced Research Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials such as metal and ceramic hot-gas filters, gas separation materials based on ceramic membranes (porous and ion transport), fuel cells, and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. In cooperation with DOE-ORO, Oak Ridge National Laboratory has the responsibility of the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research Materials Program. DOE-FE administration of the Program is through the National Energy Technology Laboratory and the Advanced Research Product Team.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

335. **FABRICATION TECHNOLOGIES FOR FUEL CELL APPLICATIONS**
$110,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
M. L. Santella (865) 574-4805

This task involves developing the materials, processes, and procedures that will be required to design and fabricate fuel cells. It directly addresses issues related to developing an economically viable Solid Oxide Fuel Cell (SOFC) system with acceptable lifetime and cost. The primary focus will be on developing and implementing joining technologies for producing the various metal-metal, ceramic-ceramic, and metal-ceramic connections required for producing cell stacks, containments, and other related structures. An immediate objective is to evaluate the use of iron aluminide alloys (Fe_3Al) for containment structures for high-temperature, solid oxide fuel cells.

Keywords: Alloys, Fuel Cells

336. **INTERMETALLIC REINFORCED Cr ALLOYS**
$110,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contacts:
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The objective of this task is to develop high-strength, oxidation- and corrosion-resistant Cr alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65% efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. These alloys are also potentially enabling in aggressive, high-temperature molten salt and slag environments, such as those encountered in gasification systems, for use in process monitoring (e.g., thermowells) and as structural components or protective coatings. The development effort will be devoted to *in situ* composite alloys based on a Cr solid solution matrix reinforced with the Cr_2X (X = Nb, Ta, ...) Laves phase.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

337. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE METALLIC ALLOYS**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli (865) 574-5119

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant Cr alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65% efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. These alloys are also potentially enabling in aggressive, high-temperature molten salt and slag environments, such as those encountered in gasification systems, for use in process monitoring (e.g. thermowells) and as structural components or protective coatings. The development effort will be devoted to *in situ* composite alloys based on a Cr solid solution matrix reinforced with the Cr_2X (X = Nb, Ta, ...) Laves phase.

Keywords: Coatings, Corrosion

338. **Mo-Si ALLOY DEVELOPMENT**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
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Oak Ridge National Laboratory Contact:
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Ames Laboratory Contact: M. J. Kramer
(515) 294-0276

The objective of this task is to develop new-generation corrosion-resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy conversion systems through increased operating temperatures, and to increase the service life of hot components exposed to corrosive environments at temperatures as high as 1600°C. This effort thus contributes directly to Vision 21, one goal of which is to significantly reduce greenhouse emissions. The effort focuses presently on Mo-Si-B alloys containing high volume fractions of molybdenum silicides and borosilicides.

Keywords: Alloys, Molybdenum, Silicon

339. **DEVELOPMENT OF MODIFIED AUSTENITIC ALLOYS**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman (865) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

340. **CRADAS ON ADVANCED ALLOY DEVELOPMENT**
$18,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman (865) 574-5108

The purpose of this task is to engage in cooperative work with industrial firms on the development of advanced austenitic alloys.

Keywords: Alloys, Austenitics, Technology Transfer

341. **CRADA ON THERMIE ALLOY PROCESSING**
$34,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman (865) 574-5108

The purpose of this task is cooperative work with Special Metals Corporation to develop the processing technology for Thermie alloy.

Keywords: Alloys, Technology Transfer

342. **CRADA WITH INCO ON HIGH CREEP STRENGTH ALLOYS**
$50,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. J. Maziasz (865) 574-5082

This activity was a collaborative work with INCO Alloys to develop high-creep-strength alloys.

Keywords: Alloys

343. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$170,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright (208) 526-6127

This program will determine the influence of processing on improved properties of alloys based on the intermetallic compound Fe_3Al. Thermomechanical processing of these alloys will be pursued to improve their ambient and elevated temperature properties. The response of the microstructure to elevated temperature deformation and subsequent annealing will be characterized in terms of the establishment of equilibrium phases, equilibrium degree of long-range order, and secondary recrystallization. Oxide dispersion strengthened (ODS) alloys fabricated by reaction synthesis will be developed for improved high-temperature strength. Tensile properties of the ODS materials will be determined at room and elevated temperature and related to the microstructure. Creep properties of these alloys will be studied in detail and compared to current theories for creep strengthening by oxide dispersions. The processing/properties relationships determined using reaction-synthesized materials will be applied to more conventional high energy ball milled ODS alloys being developed at Oak Ridge National Laboratory (ORNL). Compositions of the dispersion strengthened Fe_3Al alloys will be determined in collaboration with the program at ORNL.

Keywords: Aluminides, Processing, Microstructure

344. **EXTENDED-LIFETIME METALLIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL PROTECTION**
$210,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli (865) 574-5119

The purpose of this task is to examine important composition and microstructure issues associated with the development of extended-lifetime corrosion-resistant metallic coatings for high-temperature applications associated with the key technologies of the Office of Fossil Energy's Vision 21 concept. Two linked technical objectives support this purpose. They are 1) for a given fossil environment, establishment of the coating composition and microstructure necessary for long-term high-temperature corrosion protection and 2) determination of the relationships among composition, microstructure, and a coating method.

Keywords: Coatings, Corrosion

345. **ALUMINIDE COATINGS FOR POWER-GENERATION APPLICATIONS**
$85,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli (865) 574-5119
Tennessee Technological University Contact: Ying Zhang (931) 372-3186

The purpose of this task the fabrication, characterization and testing of aluminide coatings made on ferritic alloys such as Fe-9Cr-1Mo steels, which are being considered for use in advanced steam cycles. In addition, the influences of duty cycle length and operating temperature on the oxidation behavior of state-of-the-art bond coatings for fossil-fueled turbine engines are investigated.

Keywords: Coatings, Corrosion

346. **CHEMICALLY-VAPOR-DEPOSITED YSZ FOR THERMAL AND ENVIRONMENTAL BARRIER COATINGS**
$225,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: T. M. Besmann (865) 574-6852

The purpose of this task is to develop a chemical vapor deposition (CVD) process for fabricating yttria-stabilized zirconia (YSZ) for thermal and environmental barrier applications. YSZ has been the phase of choice for thermal barrier coating (TBC) applications due to its low thermal conductivity and high thermal stability. The CVD process being explored utilizes organometallic precursors flowing over a heated substrate in a flow reactor. A current technology for thermal barrier coatings (TBCs) for high-performance turbine blades utilizes electron-beam physically vapor deposited (EBPVD) yttria-stabilized zirconia (YSZ). The deposits are columnar in nature, resulting in excellent strain tolerance during thermal cycling. There exist, however, a number of issues with regard to cost, long-term stability, and environmental degradation of these coatings. The CVD process for YSZ is being developed for consideration as a replacement for the capital intensive EBPVD process, as a supplement to EBPVD to coat regions that the line-of-sight process cannot reach, and as a seal coat (environmental barrier coating or EBC) for EBPVD layers.

Keywords: Composites, Ceramics, Coatings

347. **CORROSION-RESISTANT COMPOSITE STRUCTURES**
$275,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: B. A. Armstrong (865) 241-5862

The purpose of this program is to develop ceramic coatings with enhanced corrosion resistance through improvements in the composition and processing of the coating. Processing innovations will focus on aqueous coating development including such techniques as spray coating, dip coating and vacuum infiltration. Approaches to coatings, such as mullite, that have shown good corrosion resistance and materials that form scales other than silica will be evaluated. Candidate materials will be exposed in facilities at ORNL, the DOE National Energy Technology Center (NETL), and the University of North Dakota Energy and Environmental Research Center (UNDEERC). All specimens will be characterized at

ORNL to identify the most promising materials for specific applications.

Keywords: Composites, Ceramics, Fiber-Reinforced, Corrosion

348. **MODELING FOR CVD OF SOLID OXIDE ELECTROLYTE**
$90,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
University of Louisville Contact: T. L. Starr (502) 852-1073

There are two critical requirements for successful, ambient pressure CVD of solid oxide electrolyte films: maintain uniformity in thickness and composition over a reasonably large substrate, and avoid gas-phase nucleation that degrades film quality. The proposed research addresses both requirements and is based on the unique characteristics of stagnation point flow.

Stagnation point flow describes the characteristics of a fluid stream impinging upon a planar substrate. With this geometry, modeling of mass and energy transport between the stream and the substrate surface can be reduced to a one-dimensional, boundary layer problem. Further, with proper selection of flow conditions, the effective boundary layer thickness is essentially uniform over an appreciable portion of the substrate. Also, by utilizing a cold-wall design—cool stream impinging on a heated substrate—the “residence time at temperature” for the stream is small, minimizing gas phase reactions.

This project shall investigate the application of stagnation point flow to the deposition of yttrium-stabilized zirconia (YSZ) solid electrolyte films, including an experimental effort at ORNL and a modeling effort at the University of Louisville.

Keywords: Ceramics, Composites, Modeling, Fuel Cells

349. **DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS**
$76,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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ReMaxCo Technologies, Inc. Contact: R. D. Nixdorf (865) 483-5060

The DOE Fossil Energy Program has an interest in silicon carbide fibrils as a material for high-temperature heat exchanger and recuperation components in advanced coal combustion plants. The purpose of this project is to develop a commercial process for the production of silicon carbide fibrils. The slow growth of the fibrils and excessive waste of raw materials have been the major impediments. This work is an effort to bring new technology solutions to the future volume production of silicon carbide fibrils.

Keywords: Ceramics, Composites, Fibrils, Modeling

350. **DEVELOPMENT OF HOT PRESSING AS A LOW-COST PROCESSING TECHNIQUE FOR FUEL CELL FABRICATION**
$4,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
Boston University Contact: Vinod Sarin (617) 353-6451

This project focuses on the development of a hot-pressing technique for fabricating the air electrode (cathode) structure, with the objective to obtain an electronically-conducting porous structure with high gas permeability and a high electronic/ionic/gas contact area. Such a structure will provide low gas-phase mass transfer resistance and low electrode-polarization resistance.

Keywords: Fuel Cells

351. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES**
$190,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous Carbon Fiber Composites (CFC) manufactured from petroleum pitch-derived carbon fibers. The Carbon Fiber Composite Molecular Sieves (CFCMS) will be utilized in Pressure Swing Adsorption (PSA) units for the efficient recovery of hydrogen from refinery purge gases, and for other gas separation operations associated with petroleum refining. Moreover, natural gas frequently contains large fractions of diluents and contaminants such as CO_2 and H_2S. CFCMS materials will be developed to effect the separation of diluents and contaminants from natural gas. Additionally, H_2O must be removed from natural gas to minimize pipeline corrosion. Novel separation techniques, that exploit the unique combination of properties of CFCMS, will be developed to effect the above-mentioned separations. The separation of air (O_2/N_2) is gaining importance because of the need for a compact separation system for vehicles powered by fuel cells. The combination of a suitably modified version of CFCMS and our electrical swing adsorption technology offers considerable potential for this application. Hence, research is being directed toward the tailoring of CFCMS for the separation of O_2/N_2.

Keywords: Carbon Fibers, Sieves, Composites

352. **CRADAS FOR DEVELOPMENT AND TESTING OF CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$107,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell (865) 576-8595

Hydrogen and methane gas recovery technologies are required to: 1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and 2) improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers.

Keywords: Carbon Products

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

353. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS**
$390,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451

The purpose of this task is to address the materials-related barriers to expediting the use of oxide dispersion-strengthened (ODS) alloys in components which are required in DOE's Office of Fossil Energy Vision 21 processes to operate at temperatures higher than are possible with conventionally-strengthened alloys. Specific goals are to develop a detailed understanding of ODS alloy behavior in all phases of their use, including fabrication, service performance, life prediction, mode of failure, repair, and refurbishment. The scope of the effort includes the development of ODS iron-aluminum alloys that combine strength levels of the same order as commercially-available ODS FeCrAl alloys, but with the superior resistance to high-temperature sulfidation and carburization attack demonstrated by the best iron aluminides. The data generated will form a resource for designers wishing to incorporate ODS alloys into components which may require modification of alloy processing to maximize strength or environmental resistance of particular forms of the alloys.

Keywords: Aluminides

354. **INVESTIGATION OF THE WELDABILITY OF INTERMETALLICS**
$70,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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Colorado School of Mines Contact: G. R. Edwards (303) 273-3773

The purpose of this project is the investigation of the weldability of polycrystalline aluminides. The major thrust of the project is to determine the role of microstructure in the intergranular cracking of aluminides, with special emphasis on weld cracking susceptibility. The weldability of polycrystalline Fe_3Al-X alloys is being evaluated, and the weldability is correlated with composition, phase equilibria, grain size and morphology, domain size, and degree of long-range order.

Keywords: Joining, Welding

355. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$20,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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I. G. Wright (865) 574-4451
West Virginia University Contact: B. R. Cooper
(304) 293-3423

The purpose of this activity is the evaluation of the intrinsic and extrinsic fracture behavior of iron aluminides and the study of atomistic simulations of defect concentrations, dislocation mobility, and solute effects in Fe_3Al. The work also involves an experimental study of environmentally-assisted crack growth of Fe_3Al at room and at elevated temperatures. The combined modeling and experimental activities are expected to elucidate the mechanisms controlling deformation and fracture in Fe_3Al in various environments.

Keywords: Alloys, Aluminides, Fracture

356. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$53,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
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Lehigh University Contact: A. R. Marder
(610) 758-4197

The objective of this activity is the investigation of iron aluminide weld overlays. Specific tasks include: 1) filler wire development 2) weldability 3) oxidation and sulfidation studies 4) erosion studies 5) erosion- corrosion studies, and 6) field exposures.

Keywords: Alloys, Aluminides, Overlay, Welding, Joining

357. **IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS**
$87,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451
Foster Wheeler Development Corporation Contact:
J. L. Blough (201) 535-2355

The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments. ORNL-modified alloys and standard comparison alloys have been examined. The variables affecting coal ash corrosion and the mechanisms governing oxide break-down and corrosion penetration are being evaluated. Corrosion rates of the test alloys are determined as functions of temperature, ash composition, gas composition, and time.

Keywords: Austenitics, Alloys, Corrosion

358. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$175,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451
Argonne National Laboratory Contact: K. Natesan
(630) 252-5103

The purposes of this task are to 1) evaluate mechanisms of oxidation, sulfidation, and breakaway corrosion in mixed gas atmospheres typical of both combustion and gasification systems 2) develop an understanding of corrosion processes that occur in ceramic materials and surface modified alloys 3) characterize the physical, chemical, and mechanical properties of surface scales that are resistant to sulfidation attack 4) evaluate the role of deposits containing sulfur and/or chlorine and ash constituents in the corrosion behavior of metallic alloys, selected coatings, and monolithic/composite ceramics, and 5) evaluate the residual mechanical properties of materials after exposure in corrosive environments and quantify the effects of corrosion on the properties to enable life prediction of components.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

359. **REDUCTION OF DEFECT CONTENT IN ODS ALLOYS**
$78,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
The University of Liverpool Contact: A. R. Jones 151-794-8026

The purpose of this work is to assess the sources of defects in oxide-dispersion-strengthened (ODS) alloys. Experiments to confirm key features of defects in ODS alloys shall be devised and performed, and recommendations shall be made for the reduction of defects in these alloys.

Keywords: Aluminides, Defects

360. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$60,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
University of North Dakota Energy and Environmental Research Center (UNDEERC) Contact: J. P. Hurley (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the Advanced Research Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: 1) hot gas cleanup systems and 2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

361. **RELIABLE CERAMIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL RESISTANCE IN FOSSIL ENVIRONMENTS**
$70,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli (865) 574-5119

The purpose of this work is to support the development of advanced ceramic-based materials for applications in fossil environments by examining critical phenomena related to high-temperature environmental resistance of ceramic coatings used to provide protection under the aggressive conditions commonly found in advanced coal-fired plants. In support of this purpose, technical objectives focus not only on chemical compatibility of standard and developmental ceramic coatings in a variety of environments, but also on their mechanical reliability.

Keywords: Coatings, Corrosion

362. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR STRUCTURAL CERAMICS**
$175,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
Argonne National Laboratory Contact: W. A. Ellingson (630) 252-5068

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens are being studied to establish correlations between NDE results and failure of specimens.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

363. **IMPERMEABLE THIN Al_2O_3 OVERLAY FOR TBC PROTECTION FOR SULFATE AND VANADATE ATTACK IN HIGH TEMPERATURE GAS TURBINES**
$333,000
DOE Contacts: F. M. Glaser (301) 903-2784 and
V. U. S. Rao (412) 386-4743
University of Pittsburgh Contact: Scott Mao
(412) 624-9602

The project focuses on one of the materials needs to demonstrate/confirm the efficacy of conventional gas turbines in a coal-derived synthesis gas system. Different hot gas environments are obtained and there is a dearth of long-term performance data for these environments. Hence a program priority is the selection and verification testing of turbine hot path component materials and protective coatings. Differences in syngas composition relative to natural gas and syngas variability due to different gasifier type must also be researched with respect to the interaction of trace contaminants with advanced turbine blade materials and coatings. Syngas contains traces of heavy metals not found in natural gas. The interactions of these trace constituents with the materials and coatings currently being used needs to be investigated. In addition, the presence of particulates may cause erosion or deposition, and gaseous species (e.g., SO_x, alkali compounds, HCl) may cause deposition and/or enhance corrosion. Synergistic effects between these various degradation processes are also likely under gas turbine operating conditions. These various potential degradation modes may be life limiting for gas turbine hot gas components (e.g., combustion chamber, vanes and blades), rather than creep and fatigue processes. Thus, protective coatings to reduce hot corrosion and to establish models to predict the lives of candidate gas turbine hot gas path materials in realistic environments for a gas turbine operating on coal-derived gases are necessary to assess potential lives of such components, and establish changes to these environments which would significantly extend these lives. Al_2O_3 overlays will be applied to single crystal superalloy turbine blade materials having TBC and bond coat consisting of YSZ/NiCrAlY. The corrosion resistance offered by the overlay deposited by two different methods, namely, sol-gel and PVD, will be evaluated in atmospheres that will simulate coal-derived gaseous fuels. Using processing-structure-property relationships, durable coating schemes will be developed.

Keywords: Gas Turbines, Thermal Barrier Coatings

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

364. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000[1]
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451

The purpose of this task is to publish a bimonthly, joint DOE-EPRI newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Materials, Components

365. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION**
$350,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572
East Tennessee Technology Park Contact:
D. E. Fain (865) 574-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

366. **PROTON EXCHANGE MEMBRANES FOR HYDROGEN SEPARATION**
$2,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Oak Ridge National Laboratory Contact:
T. R. Armstrong (865) 574-7996
Eltron Research, Inc. Contact: Shane Roark
(303) 530-0263

The objectives of this program are to develop: 1) novel designs for compact hydrogen separation membranes, 2) model the designs to determine manufacturing feasibility, 3) fabricate 1 or 2 novel membranes for testing, 4) develop reliability models for asymmetric membranes, 5)

[1]Matching funding provided by EPRI.

evaluate constrained sintering of asymmetric membranes 6) characterize materials developed by Eltron using state-of-the-art X-ray diffraction and neutron scattering analysis and 7) develop a database of materials properties of all current and past protonic conductors.

Keywords: Membranes, Separation

367. **SOLID STATE ELECTROLYTE SYSTEMS FOR FUEL CELLS AND GAS SEPARATION**
$630,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572
Pacific Northwest National Laboratory Contact:
L. R. Pederson (509) 375-2579

This project seeks to develop functional ceramic materials for applications in fossil energy conversion and gas separation. This project is composed of the following activities: 1) Stability of Solid Oxide Fuel Cell (SOFC) Materials - Aging of fuel cell materials and interfaces under high dc current loads is the principal focus of this task. Aging processes are accelerated through the use of dc currents higher than typical of an operating solid oxide fuel cell. Alternative electrolyte and electrode materials are being developed that would enable operation at reduced temperature and/or at higher efficiencies. 2) Gas Separation Using Mixed-Conducting Ceramic Membranes - Mixed ion and electron-conducting metal oxide ceramics are being developed that can be used to passively separate oxygen of high purity from air. Other uses include application as the cathode in an SOFC operating at reduced temperatures, as the membrane in a reactor to produce synthesis gas, and in the partial oxidation of hydrocarbons to produce more valuable products. This task seeks to develop promising ceramic membrane compositions and forms, to characterize the electrical, physical, and chemical properties of these ceramics, and to demonstrate applications on a laboratory scale. 3) Bismuth Oxide-Based Gas Separation Membranes - In collaboration with Oak Ridge National Laboratory (ORNL), this task will develop bismuth oxide-based solid electrolytes for use in driven oxygen separation membranes. Such compositions offer exceptionally high ionic conductivities, at least a factor of ten higher than zirconia at moderate temperatures. Research at ORNL will focus on the synthesis of alkaline earth-doped bismuth oxide electrolytes, structural characterization, and the development of processing techniques. Research at PNNL will focus on the evaluation of electrical and mechanical properties, on processing methodology, and on compatible electrode development.

Keywords: Fuel Cells, SOFC, Membranes Testing

368. **IMPROVED FUEL CELL MATERIALS AND ECONOMICAL FABRICATION**
$184,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Oak Ridge National Laboratory Contact:
T. R. Armstrong (865) 574-7996

The purpose of this project is to develop and demonstrate the capability of porous materials technology existing at the East Tennessee Technology Park as a low-cost fabrication process for the production of air electrodes for the Westinghouse Electric Company's tubular solid oxide fuel cell.

Keywords: Fuel Cells, SOFC

369. **BISMUTH OXIDE SOLID ELECTROLYTE OXYGEN SEPARATION MEMBRANES**
$125,000
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V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Oak Ridge National Laboratory Contact:
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The purpose of this task is to develop bismuth oxide-based ionic conducting solid electrolytes for use as oxygen separation membranes. To produce efficient materials which will be competitive with existing materials and processes will require experimental studies in the following areas: optimization of the crystal chemistry of the solid solutions of bismuth oxide to maximize the oxygen ion transport at moderate operating temperatures, development of processing techniques which will enhance the orientation texture of the ceramic for increased ionic transport; and characterization and evaluation of the performance of selected compositions for comparison with competing materials and technologies.

Keywords: Membranes

370. **METALLIC FILTERS FOR HOT-GAS CLEANING**
$90,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Ames Laboratory Contact: Iver Anderson (515) 294-4446

The objective of this study is to design and develop metallic filters having uniform, closely controlled porosity using a unique spherical powder processing and sintering technique. The corrosion resistance of the filter materials will be evaluated under simulated PFBC/IGCC gaseous environments in order to determine the optimum alloy composition and filter structure. The corrosion tests will also provide a means to estimate the service lives of experimental filter materials when subjected to either normal or abnormal PFBC/IGCC plant operating conditions. Metallic filters are expected to offer the benefits of non-brittle mechanical behavior and improved resistance to thermal fatigue compared to ceramic filter elements, thus improving filter reliability. Moreover, the binder-assisted powder processing and sintering techniques to be developed in this study will permit additional filter design capability (e.g., highly controlled filter porosity/permeability with greatly enhanced processing simplification), thus enabling more efficient and effective filtration.

Keywords: Filters

371. **REFRACTORY MATERIALS ISSUES IN GASIFIERS**
$100,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Albany Research Center Contact: Richard P. Walters (541) 967-5873

The purpose of this research is to characterize and understand slag component interactions with the refractories used in coal gasifiers. It is anticipated that once these interactions are understood, it will be possible to find a means of controlling, i.e., limiting, the slag-refractory interactions and extending the refractory lifetime.

Keywords: Refractories

372. **Pd-Ag MEMBRANES FOR HYDROGEN SEPARATION**
$100,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Los Alamos National Laboratory Contact: Steven A. Birdsell (505) 667-5868

The Palladium Membrane Reactor (PMR) was developed for processing tritiated water and tritiated hydrocarbons found in fusion energy, weapons, and environmental applications. In addition to these applications, the PMR has the potential to revolutionize fossil fuel processing. However, in order to use the PMR in fuel applications, further performance data and development are needed. A state-of-the-art PMR will be used to evaluate performance and determine the best operating conditions for production of pure hydrogen from coal gas. The PMR has only been tested at atmospheric pressure, whereas coal-gas processing will need to be done at higher pressures. Performance at elevated pressures will be determined. Coal gas contains impurities such as sulfur that are potentially poisonous to PMRs. This effect will be determined. Also, in order to make the technology practical for industrial use, a higher flux Pd membrane is needed. Such a membrane has been developed at Los Alamos. An advanced PMR will be constructed with the high-flux membrane and tested with simulated coal gas. Successful demonstration of the advanced PMR could lead to a radical decrease in the cost of fossil fuel processing.

Keywords: Membranes

373. **HIGH-TEMPERATURE MATERIALS TESTING IN COAL COMBUSTION ENVIRONMENTS**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
National Energy Technology Laboratory Contact: Anthony V. Cugini (412) 892-6023

Structural and functional materials used in solid- and liquid-fueled energy systems are subject to gas- and condensed-phase corrosion, and erosion by entrained particles. The material temperature and composition of the corrodents determine the corrosion rates, while gas flow conditions and particle aerodynamic diameters determine erosion rates for a given material. Corrodent composition depends on the composition of the fuel, the temperature of the material, and the size range of the particles being deposited. It is difficult to simulate under controlled laboratory conditions all of the possible corrosion and erosion mechanisms to which a material may be exposed in an energy system. Therefore, the University of North Dakota Energy & Environmental

Research Center and the U.S. Department of Energy, National Energy Technology Laboratory are working with Oak Ridge National Laboratory to provide materials scientists with no-cost opportunities to expose materials in pilot-scale systems to conditions of corrosion and erosion similar to those in occurring in commercial power systems.

NETL is operating the Combustion and Environmental Research Facility (CERF). In recent years, the 0.5 MMBtu/hr CERF has served as a host for exposure of over 60 ceramic and alloy samples at ambient pressure as well as at 200 psig (for tubes). Samples have been inserted in five locations covering 1700-2600ºF, with exposures exceeding 1000 hours. In the present program, the higher priority metals are to be tested at 1500-1600ºF in one CERF location and near 1800-2000ºF at other locations to compare results with those from the EERC tests.

Keywords: Testing

374. **MOLECULAR SIEVES FOR HYDROGEN SEPARATION**
$150,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Sandia National Laboratories Contact:
Anthony Martino (505) 844-3332

The purpose of this program is to develop and test three novel inorganic-organic materials for hydrogen separation and purification. The program will combine experimental and theoretical efforts to develop and test the following three materials as the working thin film in asymmetric Interfacial composite membranes (on alumina supports): *In situ* generated bridged polysilsesquioxanes, organic templated silicates and catalytic membranes. 1) Bridged polysilsesquioxanes belong to a class of hybrid organic-inorganic materials with thermal stability to 500°C and resistance to acids, strong bases and organic solvents. The organic bridging group can be varied to give an enormous range of materials with differing physical and chemical properties, including hydrogen permeation 2) Organic templated silicates are designed to exhibit greater thermal and chemical stability while still forming the molecular sieving layer in asymmetric membranes. These materials are prepared from silane precursors whose organic group chemically reacts during the membrane formation to generate the membrane. 3) We will team these synthetic strategies with catalyst syntheses such as micelle-mediated preparation of metal nanoclusters to generate a revolutionary catalyst separation system combining highly dispersed metal nanoclusters in hybrid membranes with precisely modulated permselectivity. These catalytic membranes will provide a technology to perform reactions such as hydrogen reforming and the water shift reaction on-line. Pure hydrogen is removed from the reaction zone with a subsequent advantage to the reaction equilibrium.

Keywords: Membranes

375. **OXIDE-DISPERSION-STRENGTHENED Fe_3Al-BASED ALLOY TUBES**
$50,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451
University of California at San Diego Contact:
B. K. Kad (619) 534-7059

The objective of this work is to explore experimental and computational means by which inherent material and processing-induced anisotropies of ODS Fe_3Al-base alloys can be exploited to meet in-service mechanical and creep-life requirements of the power generation industry. The research shall examine microscopic and microstructural issues with a view to addressing optimum material design for macroscopic components under well prescribed in-service loading criteria. The economic incentive is the low cost of Fe_3Al-based alloys and its superior sulfidation resistance, in comparison to the competing Fe-Cr-A1 base alloys and the Ni-base superalloys currently in service.

The development of suitable ODS Fe_3A1 materials and processes shall endeavor to achieve high mechanical strength at temperature, as well as prolonged creep-life in service. Post-deformation recrystallization or zone annealing processes shall be examined as necessary to increase the grain size and to modify the grain shape for the anticipated use.

Keywords: Alloys

376. **DEVELOPMENT OF ODS ALLOY FOR HEAT EXCHANGER TUBING**
$106,000
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(865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451
Special Metals Corporation Contact: Mark Harper
(304) 526-5057

This work is intended to generate information and understanding for incorporation into a database being generated by the team assembled by Special Metals Corporation to allow oxide dispersion-strengthened (ODS) alloys to be used in the design, construction, and operation of heat exchangers in the very high-temperature environments of interest in Vision 21 power plant modules. This effort has three main objectives: firstly, to characterize the effectiveness of modified processing routes aimed at optimizing the mechanical properties of the ODS-FeCrAl alloy INCO® MA956 for application as tubing. Property measurements from this activity will form part of the data package required for submission of a case for obtaining ASME Boiler and Pressure Vessel Code qualification for this alloy. Secondly, to evaluate the available techniques for joining ODS alloys, to provide a sound basis for fabrication options. The third objective is to develop a basis for service lifetime prediction based on the high-temperature oxidation behavior of this alloy.

Keywords: Alloys, Tubing

377. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-X ALLOYS**
$30,000
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(865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451
University of Tennessee Contact: P. K. Liaw
(865) 974-6356

The objective of this research is to characterize the fatigue and fracture behavior of Cr_2Nb-based alloys and other intermetallic materials at ambient and elevated temperatures in controlled environments. These studies are expected to lead to mechanistic understanding of the fatigue and fracture behavior of these alloys. Fatigue tests are conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys.

Keywords: Alloys

378. **MANAGEMENT OF THE FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM**
$400,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572

The goal of the Fossil Energy Advanced Research Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials such as metal and ceramic hot-gas filters, gas separation materials based on ceramic membranes (porous and ion transport), fuel cells, and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. In cooperation with DOE-ORO, Oak Ridge National Laboratory (ORNL) has the responsibility of the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research Materials Program. DOE-FE administration of the Program is through the National Energy Technology Laboratory and the Advanced Research Product Team.

Keywords: Management, Materials Program

379. **PERSONAL SERVICES CONTRACT**
$5,000
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The task provides funds for a personal services subcontract for services related to the preparation of exhibits for and the management of exhibits at external conferences.

Keywords: Conference, Exhibits

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC), formerly with the Bureau of Mines, incorporates Advanced Metallurgical Processes that provide essential life-cycle information for evaluation and development of materials. The research at ARC directly contributes to FE objectives by providing information on the performance characteristics of materials being specified for the current generation of power systems, on the development of cost-effective materials for inclusion in the next generation of fossil fired power systems, and for solving environmental emission problems related to fossil fired energy systems. The program at ARC stresses full participation with industry through partnerships and emphasizes cost sharing to the fullest extent possible.

The materials research in the Program focuses on extending component service lifetimes through the improvement and protection of current materials, by the design of new materials, and by defining the service operating conditions for new materials in order to ensure their safe and effective use. This process involves developing a better understanding of specific failure modes for materials in severe operating environments, addressing factors which limit their current use in these environments, and by designing new materials and materials processing procedures to overcome anticipated usage challenges in severe operating environments, such as those typically found in fossil energy generating plants and in structures and supporting facilities associated with oil and gas production. Emphasis is placed on high-temperature erosion testing and modeling in environments anticipated for Vision 21 plants, on the development of sulfidation/oxidation resistant materials which can also resist thermal cycling for pressurized circulating fluidized bed reactors, the production of low-cost titanium for use as drill strings or coiled tubing in drilling applications, and repair and development of refractory materials for coal gasifiers. DOE contact is Richard Walters (541) 967-5873.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

380. **ADVANCED FOIL LAMINATION TECHNOLOGY**
$562,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact:
Arthur V. Petty, Jr. (541) 967-5878

ARC researchers have developed a materials fabrication approach that utilizes dissimilar foils to produce a variety of materials (e.g., layered composites, monolithic metallic and intermetallic alloys). This technique has also been used to join dissimilar metals. The goal of this research is to use conventional deformation processing techniques (such as extrusion or rolling) to bond foils to substrates and to each other.

Keywords: AluminIdes, Coatings, Foil-Lamination Process

381. **CONTINUOUS CASTING OF TITANIUM**
$300,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact:
Paul C. Turner,(541) 967-5863

Nearly 50 percent of the cost of titanium can be attributed to fabrication. Currently, all wrought products are produced from cylindrical ingot which must be broken down in multiple steps of forging and rolling. The process, although more lengthy, is analogous to the same process that was once used to make wrought steel products prior to the advent of continuous casting. A similar continuous and lower cost process to prepare commercially pure titanium and titanium alloys in a variety of shapes including slab, plate, and billet would reduce costs, increase the usage of titanium, and lead to environmental benefits and energy savings. A successful conclusion of this project will result in a continuous melting and ingot making process that directly utilizes titanium sponge or scrap. Development of a melting process to produce a billet or slab surface finish that is suitable for rolling without the necessity of forging or other preparation will significantly increase yields and productivity.

Keywords: Titanium, Continuous Casting

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

382. **ADVANCED REFRACTORIES FOR GASIFIERS**
$600,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact:
Arthur V. Petty, Jr. (541) 967-5878

The emphasis of this high temperature material research has been driven by both short range industrial needs and long range issues in gasifiers. Program emphasis is on the following: 1) identifying material failure mechanisms 2) identifying/ developing materials that will extend the lifetime of primary refractory liners in slagging gasifier systems 3) developing ways to shorten system downtime caused by refractory maintenance and 4) developing improved thermocouples/temperature monitoring techniques.

Keywords: Refractories, Slagging Gasifier, Liners

383. **OXIDATION AND SULFIDATION RESISTANT MATERIALS**
$1,160,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contacts:
Arthur V. Petty, Jr. (541) 967-5878 and
Jeffrey A. Hawk (541) 967-5900

To develop modified austenitic stainless steels with performance characteristics necessary for process streams in advanced heat recovery and hot gas cleanup systems employed with advanced power generation systems (IGCC, PFBC and IGFC). The most difficult near term R&D challenges are development of hot gas particulate and sulfur cleanup systems employed with these advanced power generation systems. Primary focus is on the development of TiC-reinforced *cast* austenitic stainless steels with Al and Si additions for oxidation and sulfidation resistance.

Keywords: Alloys, Casting, Cast Austenitic Stainless Steel, Titanium Carbide

384. **EROSION AND WEAR**
$600,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact: Jeffrey A. Hawk (541) 967-5900

Wear and erosion are significant materials-related problems found in the operation of fossil energy plants. Wear is a problem in the processing of coal for use as a fuel, and erosion is a problem in the daily operation of the plant. By understanding the general wear and erosion mechanisms which occur within the plant, materials and procedures can be developed to reduce the effects of wear and erosion associated with the operation of fossil energy plants. As a result of a better understanding of these processes, developments in wear resistant materials and process designs can be made. These improvements will result in higher efficiency, less maintenance and fewer catastrophic failures in fossil energy plants. An understanding of how materials behave under conditions of impact by dry particles will be developed along the way, through understanding the contact mechanics of the impact process and by investigating and characterizing the damage inflicted on various materials by impact of particles.

Keywords: Abrasion, Erosion, Oxidation, Corrosion, Wear

385. **MECHANISMS OF CORROSION UNDER ASH DEPOSITS**
$400,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact: Jeffrey A. Hawk (541) 967-5900

Determine the influence of coal ash deposits, molten salts, and thermal gradients on the mechanisms of corrosion of alloys used in coal-fired, coal gasification, and biomass power plants.

Keywords: Corrosion, Molten Salts, Hot Corrosion

386. **NON-ISOTHERMAL CORROSION AND OXIDATION**
$200,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact: Jeffrey A. Hawk (541) 967-5900

Large temperature gradients and heat fluxes occur in turbines, heat exchangers, and walls of fossil energy power plants. The effects of temperature gradient and heat flux on oxidation, sulfidation, and hot corrosion rates and mechanisms are not well understood. The objective is to determine the effects of thermal gradients and heat fluxes on the corrosion behavior of metals commonly used in high-temperature components of fossil energy power plants. This study also examines non- isothermal oxidation and hot corrosion.

Keywords: Oxidation, Corrosion, Thermal Gradient

ULTRA-SUPERCRITICAL STEAM POWER PLANT RESEARCH

387. **MATERIALS FOR ULTRA-SUPERCRITICAL STEAM POWER PLANTS**
$299,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451

The purpose of this research is to fulfill a critical need for materials technology required to design, construct, and operate an ultra-supercritical (USC) steam boiler with much reduced heat rate and increased efficiency. Although several of the advanced materials to be used in such a boiler have been approved for construction under the rules of ASME Section I, experience with these materials is lacking with regard to fabrication of components, validity of transient analysis procedures, and specification of corrosion allowances. The research undertaken here will provide an essential database to the designers, manufacturers, and users of the USC plant.

Keywords: Materials, Power Plants

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